2010 ARO IN REVIEW

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CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Office (ARO) for fiscal year 2010 (FY10; 1 Oct 2009 through 30 Sep 2010). This report provides:

- A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- Statistics regarding basic research funding (*i.e.*, "6.1" funding) and program proposal activity
- Research trends and accomplishments of the individual ARO scientific divisions

I. ARO MISSION

The mission of ARO, as part of the U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in these disciplines: chemical sciences, computing sciences, electronics, environmental sciences, materials science, mathematical sciences, mechanical sciences, network sciences, life sciences, and physics. The goal of this basic research is to drive scientific discoveries and increase the general store of scientific knowledge through high-risk, high pay-off research opportunities primarily with universities, and also with industrial and governmental laboratories. ARO also ensures that the results of these efforts are made available to the Army research and development community, for the pursuit of long-term technological solutions for the Army.

II. ARO INVESTMENT STRATEGY

ARO emphasizes a general two-pronged investment strategy for ARO to meet its mission: *requirements pull* and *technology push*.

A. Requirements Pull

The requirements pull strategy follows classic Joint Capabilities Integrated Development System processes, in which ARO promotes research in response to a wide variety of published requirements and needs, including the Army Science and Technology Master Plan, the Training and Doctrine Command Warfighter Outcomes, and the Quadrennial Defense Review (QDR). This strategy can also be referred to as needs-driven research, which emphasizes long-term efforts to improve specific capabilities or overcoming identified technology barriers.

B. Technology Push

ARO also invests heavily in discovery research targeted at extraordinarily novel and innovative science that may not be focused on a specific application, but promises tremendous value across many technologies and applications, some of which may be fundamentally new. This technology push strategy emphasizes opportunity-driven research aimed at developing and exploiting scientific breakthroughs to produce revolutionary new capabilities.

The scope of ARO research investment strategy is broad and decidedly long range, with system applications often 10–15 years away, or more. The long-range focus of ARO's investment strategy is designed to maintain the Army's overwhelming capability in the expanding range of present and future operations. However, there have also been many research programs throughout ARO's history that had spin-offs (*i.e.*, transitions) to system applications in much shorter times, and these are actively pursued to ensure that extramural basic research is optimally contributing to the advancement of the current Warfighter's capabilities.

C. Specific Strategies

More specifically, ARO employs the following strategies to fulfill its mission:

- Execute an integrated, balanced extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage the science and technology (S&T) of other defense and government laboratories, academia and industry, and appropriate organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

III. IMPLEMENTING THE ARO INVESTMENT STRATEGY

As described in the previous section, ARO employs multiple strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

A. Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator initiatives. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs (see CHAPTER 2-IX). The National Defense Science and Engineering Graduate (NDSEG) fellowship program is one mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation (see CHAPTER 2-X). ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists (see CHAPTER 2-XI). In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see CHAPTER 2-VIII).

B. Coordination for Program Development and Monitoring

The research programs and initiatives that compose ARO's extramural research program are formulated through an ongoing and active collaboration with a variety of Federal research organizations, including the:

- ARL Directorates:
  - Computational and Information Sciences Directorate (ARL-CISD)
  - Human Research and Engineering Directorate (ARL-HRED)
  - Sensors and Electron Devices Directorate (ARL-SEDD)
  - Survivability/Lethality Analysis Directorate (ARL-SLAD)
  - Vehicle Technology Directorate (ARL-VTD)
  - Weapons and Materials Research Directorate (ARL-WMRD)
- Research, Development, and Engineering Centers (RDECs) within the Research, Development and Engineering Command (RDECOM)
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command

While the Army Material Command's RDECOM is the primary user of the results of the ARO research program, ARO also supports research of interest to the Army Corps of Engineers, MRMC, other Army Commands, and DoD agencies. Coordination and monitoring of the ARO extramural program by the ARL Directorates, RDECs, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University Affiliated Research Centers (UARCs) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates, RDECs, and other DoD, academic, and industry representatives who serve on evaluation panels for each university center.

Office of the Secretary of Defense (OSD) research programs that are managed by ARO include the University Research Initiative (URI) programs, HBCU/MI, and NDSEG programs. These programs also fall under the executive oversight of the Defense Basic Research Advisory Group. Other members of this group include the Assistant Secretary of Defense for Research and Engineering (ASDR&E), formerly known as the Director, Defense Research and Engineering (DDR&E), and representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR) and the Defense Advanced Research Projects Agency (DARPA).

CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's premier extramural basic research agency in the physical, engineering, life, and information sciences. ARO implements these investment strategies through research programs and initiatives that together make up ARO's extramural research effort. These programs each have unique objectives and eligibility requirements and receive funding from a variety of DoD sources. This chapter describes the visions, objectives, and funding sources of these programs, which compose the overall ARO extramural research program.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO according to scientific discipline (*e.g.*, chemical sciences). ARO's Divisions are aligned with these disciplines and each has its own vision and research objectives as described in CHAPTERS 3-12. Each Division identifies topics that are included in the broad agency announcement (BAA). These topics encourage researchers to submit white papers and proposals in areas that support the Division's objectives.

I. OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as discussed in the following subsections.

A. Army Funding

The majority of the extramural basic research programs managed by ARO is funded by the Army. These programs are indicated below and are described in more detail later in this chapter.

- The Core (BH57) Research Program, funded through basic research "BH57" funds (see Section II).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program (see Section III)
  - Presidential Early Career Awards for Scientists and Engineers (PECASE; see Section IV)
  - Defense University Research Instrumentation Program (DURIP; see Section V)
- Two University Affiliated Research Centers (UARCs; see Section VI)
- The Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see Section VIII)

ARO coordinates with the Office of the Secretary of Defense (OSD) in the management of Army-funded URI programs (MURI, PECASE, and DURIP).

B. Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed by ARO are provided by OSD. The objectives for these programs are described in later sections of this chapter.

- Infrastructure Support Program (ISP) for Historically Black Colleges and Universities and Minority Institutions (HBCU/MI; see Section IX)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships (see Section X)
- Youth Science Activities (see Section XI)

These activities are mandated by DoD's Chief Technology Office, the Assistant Secretary of Defense for Research and Engineering (ASDR&E), formerly known as the Director, Defense Research and Engineering (DDR&E). Each of these OSD-funded programs has a different focus and/or different target audience. ARO has

been designated by ASDR&E as the lead agency for the implementation of ISP for HBCU/MI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

In FY10, the Defense Experimental Program to Stimulate Competitive Research (DEPSCoR) program officially ended, as DoD no longer included this effort in fund requests for FY10 and future year budgets.

C. Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (*e.g.*, Defense Advanced Research Projects Agency [DARPA] and Defense Threat Reduction Agency [DTRA]) to support a variety of external programs with specific research focuses. These joint programs have research objectives in line with the investment strategies of both an ARO Division and the strategies of the funding source or partner agency. Due to the unique nature of these cooperative efforts and their alignment with a specific scientific discipline, each externally-funded effort is discussed within the chapter of the scientific Division with which they align (see CHAPTERS 3-12).

II. ARO CORE (BH57) RESEARCH PROGRAM

ARO's Core Research Program is funded with Army basic research "BH57" funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, environmental, life, materials, mathematical, mechanical, and network sciences. The goals of this program are to utilize world-class and worldwide academic expertise to discover and exploit novel scientific opportunities, primarily at universities, to address the Army's 2010 Modernization Strategy.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards, (b) Short Term Innovative Research efforts, (c) Young Investigator Program, (d) support for conferences, workshops, and symposia, and (e) special programs. A summary of the FY10 Core Research Program (Project BH57) funding is presented in TABLE 1. The FY10 Core Program proposal actions, according to scientific Division, are presented in TABLE 2.

A. Single Investigator (SI) Program

The goal of the SI program is to pursue some of the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continually-open BAA solicitation. All states are eligible to receive funding within this program, which focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk, initial proof-of-concept ideas, typically within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal within another program, to be evaluated for potential longer-term funding options, such as an SI award.

C. Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty members to Army research, to support their research, and to encourage their teaching and research careers. Young investigators meeting eligibility requirements may submit a YIP proposal. Outstanding YIP projects may be considered for the prestigious PECASE award (see Section IV).

D. Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical conferences that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation.

E. Special Programs

Although the ARO SI, STIR, YIP, and conference-support programs constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. These special programs include the Army Supported High School Apprenticeship Program (HSAP), which is part of the Youth Science Activities (see Section XI), funding for in-house staff and research activities, and matching funds applied to the OSD-funded HBCU/MI program.

F. Summary of FY10 ARO Core Program Funding and Actions

TABLE 1 lists the FY10 ARO Core (BH57) Program funds allocated to ARO Divisions and special programs. The FY10 Core BAA research proposal actions, according to scientific Division, are presented in TABLE 2.

TABLE 1

ARO Core (BH57) Program FY10 funding. Listed first are the FY10 ARO Core Program funds allocated to each scientific discipline/Division (for projects in the SI, STIR, YIP, and conference categories), followed by the Core Program funds allocated to various special programs.

ARO Core (BH57) Program Type	Division or Program Title	FY10 Allotment
Scientific Disciplines	Chemical Sciences	$5,422,000
	Computing Sciences	$2,882,821
	Electronics	$4,676,722
	Environmental Sciences	$2,446,055
	Life Sciences	$5,361,312
	Materials Science	$4,925,317
	Mathematical Sciences	$3,585,400
	Mechanical Sciences	$4,670,025
	Network Sciences	$4,196,850
	Physics	$5,103,700
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$43,270,202**
Special Programs	Senior Research Scientist Research Programs*	$2,852,550
	National Research Council (NRC) Associates Program	$450,000
	HBCU/MI Program**	$1,100,000
	Army-supported High School Apprenticeship Program (HSAP)	$150,000
	In-House Operations	$15,047,248
	SUBTOTAL: Core Program Funding to Special Programs	**$19,599,798**
TOTAL	**ARO Core (BH57) Program**	**$62,870,000**

* Includes Directorate-level funding

** Core program funds match OSD funds allocated to this program

TABLE 2

FY10 ARO Core (BH57) Program proposal actions. ARO Core Program projects are funded through Army BH57 funds and can include SI projects, STIR efforts, YIP projects, and support for conferences, workshops, and symposia. The sum of the proposals accepted, rejected, or withdrawn does not always equal the number received because proposal actions are not necessarily completed during the year of receipt.

	Received*	Accepted*	Declined	Withdrawn
Chemical Sciences	90	57	25	3
Computing Sciences	39	21	23	0
Electronics	57	40	6	0
Environmental Sciences	44	31	7	1
Life Sciences	68	48	16	1
Materials Science	37	29	19	0
Mathematical Sciences	37	17	14	1
Mechanical Sciences	49	37	24	3
Network Sciences	34	27	9	1
Physics	25	15	24	0
Tech Integration and Outreach	2	1	1	0
TOTAL	**482**	**323**	**170**	**10**

* The "Received" column lists only proposals submitted to the ARO Core Program BAA (including SI, STIR, YIP, and conference proposals); however, some proposals that were accepted were funded through leveraged (*i.e.*, non-BH57) sources, such as customer funds. Therefore, proposals listed in the "Accepted" column can include projects supported through a variety of funding sources.

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

As described in Section I: *Overview of Program Funding Sources*, the MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional science and engineering discipline. A multidisciplinary team effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD.

In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts intersect more than one traditional research specialty, and are typically funded at $1.25M per year for five years. These "critical mass" efforts are expected to enable more rapid research and development (R&D) breakthroughs and to promote eventual transition to Army applications.

Management oversight of the MURI program comes from the Research Office of ASDR&E to the Service Research Offices (OXRs), where OXR program managers manage the MURI projects. The OXRs include ARO, the Air force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR program managers have significant flexibility and discretion in how the individual projects are monitored and managed, while ASDR&E defends the program to higher levels in OSD and has responsibility for overall program direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by ASDR&E under a formal acquisition process.

The following topics resulted in ten newly-funded Army MURI awards for FY10. The program managers (PMs) and corresponding scientific division for each award are listed following the award titles.

1. *Neuronal Behavior in Primary Blast*, Dr. Elmar Schmeisser, Life Sciences and Dr. Bruce LaMattina, Mechanical Sciences
2. *Identifying and Extracting the Mathematical Signatures of Prokaryotic Activity in DNA; Developing a Theoretical Foundation for Predicting DNA Stability*, Dr. Mimi Strand, Life Sciences; Dr. Janet Spoonamore, Network Sciences and Dr. Wallace Buchholz, Life Sciences
3. *Tomography of Social Networks of Asymmetric Adversaries*, Dr. John Lavery, Mathematics
4. *Adaptive Perception and Agile Autonomy in Severe Environments*, Dr. Randy Zachery, Network Sciences
5. *Structured Modeling for Low-Density Languages*, Dr. Joseph Myers, Computing Sciences
6. *Directed Self-Assembly of Reconfigurable Materials*, Dr. John Prater, Materials Science and Dr. Douglas Kiserow, Chemical Sciences
7. *Atomtronics: A Generalized Electronics*, Dr. Marc Ulrich, Physics
8. *Bio-Electronic Templates for Interfacing to the Nanoscale*, Dr. Dwight Woolard, Electronics and Dr. Richard Hammond, Physics
9. *Ion Transport In Complex Heterogeneous Organic Materials*, Dr. Robert Mantz, Chemical Sciences and Dr. David Stepp, Materials Science
10. *Defect Reduction in Superlattice Materials*, Dr. William Clark, Electronics, Dr. John Prater, Materials Science and Dr. Marc Ulrich, Physics

The following topics were published in the FY11 MURI BAA. The PMs for each topic are listed following the topic titles.

1. *Controlling the Abiotic/Biotic Interface*, Dr. Jennifer Becker, Chemical Sciences and Dr. Stephanie McElhinny, Life Sciences
2. *Quantum Stochastics and Control*, Dr. Harry Chang, Mathematical Sciences and Dr. TR Govindan, Physics
3. *Qubit Enabled Imaging, Sensing and Metrology,* Dr. TR Govindan, Physics and Dr. Harry Chang, Mathematical Sciences
4. *Flex-Activated Materials*, Dr. David Stepp, Materials Science and Dr. Douglas Kiserow, Chemical Sciences
5. *Game Theory for Adversarial Behavior*, Dr. Purush Iyer, Network Sciences and Dr. Harry Chang, Mathematics
6. *Light Filamentation*, Dr. Richard Hammond, Physics
7. *Novel Free-Standing 2D Crystalline Materials (Oxides/Nitrides)*, Dr. Pani Varanasi, Materials Science
8. *Value of Information for Distributed Data Fusion*, Dr. Liyi Dai, Computing Sciences

IV. PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to outstanding scientists and engineers beginning their independent careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology (S&T) that is relevant to the mission of the sponsoring organization or agency, and (ii) community service demonstrated through scientific leadership, education, or community outreach. ARO initiated five new PECASE awards in FY10.

V. DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new university capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase scientific equipment costing $50K or more to conduct DoD-relevant research. The research is consistent with the Army Science and Technology Master Plan (ASTMP) and the 2010 Army Modernization Strategy. In mid-FY10, DoD made 166 awards to 96 academic institutions with awards ranging from about $50K to $930K with an average award amount of $235K. Of the total, the Army awarded 69 awards at $9.9M total, with the average award being $143K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCS)

The University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by DDR&E (currently ASDR&E), OSD in order to advance DoD operations by pursuing leading-edge basic research and to maintain core competencies in specific domains (unique to each UARC), for the benefit of DoD components and agencies. One DoD Service or Agency is formally designated by ASDR&E to be the primary sponsor for each UARC. The primary sponsor ensures the DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD.

ARO is the primary sponsor for two UARCs:

- The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT). The ISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Institute for Collaborative Biotechnologies (ICB) located at the University of California, Santa Barbara, with academic partners at MIT and the California Institute of Technology (Caltech). The ICB is discussed further in CHAPTER 7: LIFE SCIENCES DIVISION.

VII. MINERVA RESEARCH INITIATIVE

The Minerva Research Initiative is a DoD-sponsored, university-based social science research program initiated by the Secretary of Defense. It focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social science community. Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD. Minerva projects are funded up to a five-year base period with one five-year renewal option, with a typical award funded in the range of $1.0–1.5M per year.

VIII. SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established SBIR and STTR programs in 1982 and 1994, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen and broadly administered by the Office of Small Business Programs within the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics. The Army-wide SBIR Program is managed by RDECOM, while the Army-wide STTR Program is managed by ARO.

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) increase small business participation in federal R&D, (iii) increase private sector commercialization of technology developed through federal R&D, and (iv) foster and encourage participation in federal R&D by businesses that are owned by women and socially and economically disadvantaged individuals. The STTR program has the additional requirement that small companies must partner with an academic or other qualifying non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

B. Three-phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 3.

TABLE 3

Three-phase process of the SBIR and STTR programs. These programs employ a three-phase structure. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	• 6 months, \$70K – \$150K max • 4-month option (at Government's discretion), \$50K max, to fund interim Phase II efforts	• 6 months, \$100K max • No options
Phase II	• 2 years, \$1M max	• 2 years, \$750K
Phase III	• No time or size limit • No SBIR funds	• No time or size limit • No STTR funds

1. Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR solicitation contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the solicitation, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

2. Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (*i.e.*, a technology, product, or service). The Phase II selection process is also highly competitive. Successful Phase I contractors are invited to submit Phase II proposals as there are no separate Phase II solicitations. Typically 50% of Phase II proposals are selected for award. Phase II awards may also be selected to receive additional funds as a fast track (Phase II-FT) or Phase II Enhancement.

3. Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets.

C. Contract Awards

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, and CBD-SBIR topics that are published during specific solicitation periods throughout each fiscal year. Proposals are evaluated against

published evaluation criteria and selected for contract award. Contract awards in the SBIR and STTR programs are made pending completion of successful negotiations with the small businesses and availability of funds. The total FY10 funding for ARO-managed SBIRs, CBD-SBIRs, and STTRs is shown in TABLE 4.

TABLE 4

FY10 funding for ARO-managed SBIR and STTR contracts. FY10 funding for ARO-managed SBIR and STTR contracts including Army, OSD, and other DoD funding sources.

	SBIR Contracts FY10 Funding	STTR Contracts FY10 Funding
Phase I	$817K	$2,499K
Phase II	$4,159K	$11,471K
TOTAL	**$4,976K**	**$13,970K**

IX. HISTORICALLY BLACK COLLEGE AND UNIVERSITIES AND MINORITY INSTITUTIONS (HBCU/MI) PROGRAMS

Programs for HBCU/MIs are a significant part of the ARO portfolio. Historically, total funding for the HBCU/MI programs has collectively exceeded $38M, but totaled approximately $57.5M in FY10, including funding for programs that were awarded in FY10 and programs that were programmed for FY10 and will be awarded in early FY11.

Throughout FY09 and into FY10, HBCU/MI funding was impacted by the U.S. Court of Appeals for the Federal Circuit ruling in the case Rothe Development Corporation vs. the U.S. DoD and the U.S. Department of the Air Force. In short, the court ruled that 10 U.S.C. 2323, the basis for set aside of funding for some HBCU/MI Programs, was unconstitutional and therefore could not be used to fund such institutions exclusively. The programs administered by ARO on behalf of ASDR&E and the Partnership in Research Transition (PIRT) Program were notably delayed in execution because of this ruling. However, in FY10, set-aside programs for HBCU/MIs resumed under new authority provided by Section 252 of the National Defense Authorization Act for FY10 (enacted in 10 U.S.C. 2362) and with funding provided in the DoD Appropriations Act, 2010. These were executed under policy and guidance of the Under Secretary of Defense (Acquisition, Technology & Logistics), the Basic Science Office within the Research Directorate of ASDR&E and the Office of the Assistant Secretary of the Army (R&T). The ARO (Core) HBCU/MI Program continued throughout the year without interruption.

ARO was selected to administer the Congressionally-directed program "Iraq/Afghanistan War Veterans Training Program" for an HBCU institution located in South Carolina. Funding for this FY10 statutory add totals approximately $1.98M. In addition, the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve more than twenty scholars during FY10.

During FY10, solicitations were published for covered institutions: (i) Tribal Colleges and Universities (TCU), (ii) Research and Educational Program for HBCU/MI, and (iii) Partnership in Research Transition (PIRT) Program. These programs are discussed in the following subsections, as is the ARO (Core) HBCU/MI Program, which is part of ARO's BAA.

A. ARO (Core) HBCU/MI Program

The ARO began its HBCU/MI program in 1980 with $0.5M designed to encourage greater participation of HBCUs and MIs in basic research. The initiative has continued and in recent years has been funded at $1.2M annually. These funds are made available to the ARO scientific divisions as co-funding opportunities to support

HBCU/MI research proposals submitted under the ARO Core Program BAA. In FY10, the ARO HBCU/MI program supported 25 grants and 4 conferences with a total value of approximately $2.5M. The HBCU/MI institutions funded under the ARO Core program were afforded the opportunity to submit add-on proposals to fund high school student research apprenticeships under the newly established High School Apprenticeship Program (HSAP). Eight institutions were funded under HSAP totaling approximately $45,440. More information on HSAP can be found in Section XI: *Youth Science Activities*.

B. Partnership in Research Transition (PIRT) Program

The PIRT Program is established as the second phase of what was previously known as the Battlefield Capability Enhancement Centers of Excellence (BCE). The program's objective is to enhance the programs and capabilities of a select number of high-interest scientific and engineering disciplines through Army-relevant, topic-focused, near-transition-ready innovative research. Furthering ARL's policy of advocating and supporting research at HBCUs, and consistent with the stated mission of the White House Initiative on HBCUs, a secondary objective of PIRT is "to strengthen the capacity of HBCUs to provide excellence in education" and to conduct research critical to DoD national security functions. Funding for this program totals approximately $2.5M per year. A total of 22 research proposals were received from 12 HBCUs and awards are anticipated to be made during the second quarter of FY11. Approximately $2M was competitively awarded to HBCU institutions that conducted research through a BCE Center and MSI partners in Collaborative Technology Alliances through submission of proposals to the ARO Core BAA. Seven institutions were awarded grants ranging from $100K to $500K.

C. DoD HBCU/MI Programs

ARO has administered programs on behalf of ASDR&E (formerly DDR&E) since 1992. During FY10, approximately $45M was made available for new awards under the solicitation "*Research and Educational Program for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI)*." This program aims to: (i) enhance programs and capabilities in scientific and engineering disciplines critical to the national security functions of the DoD, (ii) encourage greater participation in DoD programs and activities, (iii) increase the number of graduates, including underrepresented minorities, in the fields of science, technology, engineering and/or mathematics (STEM), and (iv) encourage research and educational collaboration with other institutions of higher education directed toward advancing the state of the art and increasing knowledge.

Under this program, covered institutions were able to submit proposals to compete for Centers of Excellence (three focused on STEM education and three focused on STEM research) and approximately 25 basic research proposals. Proposals were received in late FY10 and awards are anticipated to be made in second quarter FY11.

D. DoD Instrumentation Program for Tribal Colleges and Universities (TCUs)

As Congressional set-aside program for TCUs, this instrumentation program aims to enhance science, mathematics, and/or engineering education programs and/or research capabilities through the acquisition of equipment and/or instrumentation that will augment existing facilities, enhance curricula, or help develop new laboratories, programs and capabilities in these areas. This includes basic equipment for laboratory and classroom use as well as sophisticated instruments and computers (including software) for advanced studies and research important to DoD. Fifteen proposals were submitted in response to the solicitation and thirteen were selected, for awards totaling approximately $3.5M. It is anticipated that awards will be made in 1Q FY11.

X. NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is an OSD-funded program administered by AFOSR, designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with ONR, AFOSR, and the DoD High Performance

Computing Modernization Program. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships last for three years, and Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend, and up to $1K/year in medical insurance.

With approximately $5M available to the Army in FY10, ARO selected 63 NDSEG Fellows from eleven categories relevant to the Army fundamental research priorities. These awardees began their fellowships in the fall of 2010. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. The number of Fellows chosen from each discipline was based on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY10 NDSEG program is shown in TABLE 5.

TABLE 5

FY10 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY10, according to the eleven topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY10
Biosciences	13
Chemistry	7
Physics	6
Computer and Computational Sciences	6
Mathematics	4
Aeronautical and Astronautical Engineering	4
Civil Engineering	2
Electrical Engineering	7
Geosciences	2
Materials Science and Engineering	5
Mechanical Engineering	7
TOTAL	**63**

XI. YOUTH SCIENCE ACTIVITIES

ARO Youth Science Programs are sponsored by the Army and have one purpose in common: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring tutorial classes during the summer, showcasing talented young high school scientists at symposia, and student science fair support.

The Army's programs for the youth of this nation collectively reach more than 100,000 high school students throughout the United States, Puerto Rico, and DoD Schools of Europe and the Pacific. Students participating in the programs during this past fiscal year were awarded more than $380K in college tuition scholarships, savings bonds totaling in excess of $30K, and expense-paid trips to international programs.

During the summer of FY10, 187 students served as interns and worked in university laboratories with selected mentors though the High School Apprenticeship Program (HSAP) and the Research and Engineering Apprenticeship Program (REAP). More than 400 students participated in programs that offered enrichment

classes in STEM through the Un-initiates' Introduction to Engineering (UNITE) program. Over 330 additional students learned engineering and alternative energy concepts as they designed, built, and raced solar cars through JSS. These programs are described further in the following subsections.

A. Junior Science and Humanities Symposium (JSHS) Program

The JSHS Program promotes original research and experimentation in the sciences, engineering, and mathematics at the high school level and publicly recognizes students for outstanding achievement. By connecting talented students, their teachers, and research professionals at affiliated symposia and by rewarding research excellence, JSHS aims to widen the pool of trained talent prepared to conduct research and development vital to our nation. Forty-eight regional symposia are conducted throughout the U.S. and DoD schools in Europe and the Pacific. Top student winners from each region are invited to attend the national symposium, hosted by ARL in Bethesda, Maryland in 2010. Approximately 8,800 students participate in JSHS through submission of research papers in the regional and national symposia.

B. Research and Engineering Apprenticeship Program (REAP)

REAP is designed to offer historically under-represented high school students the opportunity to expand their background and understanding of scientific research. This is accomplished by offering the student an internship during the summer months to participate in a work/study atmosphere with a mentor in a laboratory setting. The experience serves to motivate the student towards a career in STEM by providing a challenging science experience that is not readily available in high school.

C. Un-initiates' Introduction to Engineering (UNITE) Program

The UNITE Program is an aggressive and effective initiative that encourages and assists under-represented students in preparing for entrance into engineering schools. High school students are provided the opportunity during the summer months to participate in college-structured summer courses that provide hands on applications, participation in lectures, problem solving as well as tours of laboratories and private and governmental engineering facilities. The students are introduced to ways in which math and science are applied to real-world situations and demonstrates how they are related to careers in engineering and technology. Eight sites were funded in FY10 serving more than 500 students.

D. International Science and Engineering Fair (ISEF) Program

The ISEF Program provides high school students the opportunity to present their projects, in competition with their peers, to Army judges who are special award sponsors at these annual events. Each year, ROTC units, Recruiting Battalions, Army Reservists, and Army command/laboratory personnel serve as judges of student projects at more than 275 science fair competitions held throughout the United States and Puerto Rico. By participating in science fairs, the Army is able to encourage and stimulate talented students to consider careers in science and technology while simultaneously exposing these students to Army R&D opportunities.

E. Junior Solar Sprint (JSS) Program

The JSS Program provides 4^{th}-8^{th} grade students in the northeast an opportunity to learn engineering and renewable energy concepts and apply them by building and racing solar cars. Students form teams in their local communities, build solar cars with the help of trained mentors, and race them in local competitions. Top winners from each local competition are invited to race in the Northeastern championship in Springfield, MA.

F. High School Apprenticeship Program (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in a university structured research environment under the direction of existing ARO-sponsored principal investigators (PI) serving as mentors. FY10 marked the pilot year of the HSAP, with 50 apprentices participating at 26 different universities. The ARO invested approximately $170K in the pilot effort.

G. Youth Science Cooperative Outreach Agreement (YS-COA)

The YS-COA was awarded on 30 September to provide support and stimulation of STEM education and outreach in conjunction with DoD and the Army. YS-COA brings together government and a consortium of organizations working collaboratively to further STEM education and outreach efforts nationwide and consists of twelve major components, including the existing ARO Youth Science portfolio (JSHS, REAP, UNITE, JSS, and ISEF), the Science and Engineering Apprentice Program (SEAP), College Qualified Leaders (CQL), Gains in the Education of Mathematical Sciences and Science (GEMS), ECybermission Internship Program (ECIP), ARL Intern Program, Teach the Teacher, and a strategic overarching marketing and metrics collection effort.

Virginia Polytechnic Institute and State University will lead the consortium of non-profits and academic institutions to execute a collaborative STEM education and outreach program that focuses on the following core objectives.

- Increase the number of STEM graduates to address the projected shortfall of scientists and engineers in National and DoD positions
- Expand the involvement of students in ongoing DoD research
- Provide STEM educational opportunities for students at all stages of their K-12, undergraduate, graduate, and post-graduate education
- Entice students into college-level DoD programs
- Inform students about military or civil service career opportunities in STEM

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, all branches of the military, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academicians working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide the government sponsors with scientific and technical results and solutions to problems related to research and development by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Chapel Hill Operations office located in Chapel Hill, North Carolina on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration and technical performance of all work conducted under the program. Over the past 37 years, BMI has administered and managed over 13,000 tasks supporting critical scientific and technical needs in many agencies within the federal government.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY10, in addition to the more traditional use of the program, new tasks were initiated to support Warfighters and Combatant Commanders engaged in the Global War on Terror, Operation Iraqi Freedom, and Homeland Security.

In FY10, there were a total of 223 new SSP tasks awarded and a modification of the scope and/or funding of 395 ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY10 new SSP tasks is provided in TABLE 6.

TABLE 6
FY10 SSP tasks and sponsoring agencies.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	23
Army Research Office (ARO)	8
Edgewood Chemical Biological Center (ECBC)	3
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	7
Armaments RDEC (ARDEC)	16
Communications-Electronics RDEC (CERDEC)	11
Natick Soldier RDEC (NSRDEC)	6
Tank Automotive RDEC (TARDEC)	12
TOTAL: RDECOM	**86**
Army Medical Research and Materiel Command (MRMC)	
Aeromedical Research Laboratory (AARL)	8
Medical Research Institute of Chemical Defense (ICD)	6
Medical Research Institute of Infectious Diseases (IID)	1
Walter Reed Army Institute of Research (WRAIR)	22
TOTAL: MRMC	**37**
Other DoD	
Office of Secretary of Defense (OSD)	3
Headquarters Department of Army (HQ DA)	2
Army Training and Doctrine Command (TRADOC)	1
Army Corps of Engineers	30
Marine Corps	1
Navy	21
Air Force	15
Miscellaneous DoD	12
TOTAL: Other DoD	**85**
Department of Health & Human Services (DHHS)	7
Department of Homeland Security (DHS)	4
Department of Commerce (DoC)	1
National Aeronautics and Space Administration (NASA)	1
National Security Agency (NSA)	2
TOTAL FY10 SSP Tasks	**223**

XIII. PROGRAM FUNDING SUMMARY

Summaries of the funding sources and FY10 allotments for programs managed or co-managed with ARO are provided in TABLES 7-10.

TABLE 7

FY10 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 1, represent all of the Army-funded programs managed through ARO.

Other Army-funded Programs	FY10 Allotment
Multidisciplinary University Research Initiative (MURI)	$55,000,496
Presidential Early Career Award for Scientists and Engineers (PECASE)	$4,870,000
Defense University Research Instrumentation Program (DURIP)	$10,370,004
University Research Initiative (URI) Support	$1,611,000
MINERVA Program (Projects V72 and D55)	$5,519,500
Strategic Technology Initiatives (STI)	$375,000
Army Center of Excellence	$958,000
Institute for Collaborative Biotechnologies (ICB)	$8,251,000
HBCU/MI – Battlelab Centers	$2,638,000
Institute for Creative Technologies (ICT)	$7,486,000
Institute for Soldier Nanotechnologies (ISN)	$9,862,000
Board of Army Science and Technology (BAST)	$1,144,000
Small Business Technology Transfer (STTR)	$13,970,315
Small Business Innovation Research (SBIR)	$7,550,599
ARO-W Ballston Lease	$65,000
Youth Science Activities	$2,335,500
Research In Ballistics	$903,000
SBIR Support Services/Performance Results Corp. Contract Support	$1,150,000
TOTAL: Other Army-funded Programs	**$134,059,414**

TABLE 8

FY10 allotments for externally-funded programs. FY10 funds received from sources other than Army or OSD are indicated below. Note that in prior years of ARO in Review, this data was reported in combination with the data shown in TABLE 8. The other customer funds category includes funding from a variety of customer sources, such as the Joint IED Defeat Organization (JIEDDO) and the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC).

External Program	FY10 Allotment
Defense Advanced Research Projects Agency (DARPA)*	$134,035,184
Scientific Services Program (SSP)	$54,813,205
Chief of Staff of the Army	$ 57,231,809
National Security Agency (NSA)	$17,269,335
Defense Threat Reduction Agency (DTRA)	$13,651,420
Simulation and Technology Training Center	$10,428,501
Army Medical Research Acquisition Activity	$6,757,230
Other Customer Funds (*e.g.*, JIEDDO and JPMNBC)	$50,308,497
TOTAL: External Programs	**$344,495,181**

* Includes FY09 DARPA funds received in FY10

TABLE 9

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Note that OSD provides a portion of the total SBIR and HBCU/MI program funding and the funds reported here are FY10 funds received within FY10 (1 Oct 2009 – 30 Sep 2010).

OSD Direct-funded Programs	FY10 Allotment
OSD Small Business Innovation Research (SBIR)*	$2,279,515
OSD Historically Black Colleges and Universities/Minority Institutions (HBCU/MI)*	$53,220,000
OSD Chemical and Biological Defense (CBD) Programs	$9,608,222
TOTAL: OSD Direct Funding	**$65,107,737**

*OSD is only one funding source for the total SBIR program funds

TABLE 10

FY10 congressional add-on funding. In accordance with congressional directives, ARO identifies and manages funding to research efforts in support of specific congressional incentives, as listed in the table.

Congressional Adds	FY10 Allotment
Perpetually Assailable and Secure Information Systems *(Carnegie Mellon Univ.)*	$3,182,000
Cyber Threat Analytics *(Metaflows, Inc.)*	$2,388,000
Secure Open Source Initiative *(North Carolina State Univ.)*	$2,388,000
Maine Center for Toxicology and Environmental Health, Toxic Particles Research and Equipment *(Univ. of Southern Maine)*	$1,592,000
Lightweight Polymer Designs for Soldier Combat Optics *(Fosta-Tek Optics, Inc.)*	$796,000
Bioactive Polymers and Coating Systems for Protection Against Bio-threats *(North Dakota State Univ.)*	$3,581,000
Understanding Blast-Induced Brain Injury *(Diversified Technology, Inc., and Univ. of Nebraska)*	$2,387,000
Security Protection Using Ballistic Core Technology *(Tex Tech Industries, Inc.)*	$3,900,000
Cooperative Developmental Energy Program *(Fort Valley State Univ.)*	$1,592,000
Manufacturing Lab for Next Generation Engineers *(Bradley Univ.)*	$1,592,000
Development of Enabling Technologies for Power from Green Sources *(Univ. of Massachusetts)*	$1,194,000
Manufacturing and Industrial Technology Center *(Tallahassee Community College)*	$398,000
Academic Support and Research Compliance for Knowledge Gathering *(Univ. of Kansas)*	$1,990,000
Adv. Polymer Systems for Defense Applications: Power Generation, Protection, and Sensing *(Missouri Univ. of Science and Tech.)*	$2,387,000
TOTAL: Congressional Adds	**$29,367,000**

TABLE 11
Summary of FY10 funding. This table lists the subtotals from previous tables (TABLE 1 and TABLES 7-10).

Program Category	FY10 Funds
Core (BH57) Programs	$62,870,000
Other Army-funded Programs	$134,059,414
External Program Funds	$344,495,181
OSD Direct-funded Programs	$65,107,737
Congressional Adds	$29,367,000
GRAND TOTAL: FY10 Funds (all sources)	**$635,899,332**

CHAPTER 3: CHEMICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Chemical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research efforts to advance the Army and nation's knowledge and understanding of the fundamental properties, principles, and processes governing molecules, and their interactions in materials or chemical systems. More specifically, the Division promotes basic research studies to uncover the relationships between macromolecular architecture and material properties, to understand the fundamental processes governing electrochemical reactions, to develop methods for accurately predicting the pathways, intermediates, and energy transfer of specific reactions, and to discover and characterize the many chemical processes that occur at surfaces. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of chemical sciences research. In addition, these efforts will likely reveal new methods for synthesizing and analyzing molecules and materials that will open the door to future studies that are not feasible with current methods.

2. Potential Applications. In addition to advancing world-wide knowledge and understanding of chemical processes, research efforts managed in part through the Chemical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by research in the chemical sciences could provide materials with new or enhanced properties to protect the Soldier from ballistic, chemical, and biological threats. The development of new computational methods may allow the structure and properties of notional (*i.e.*, theoretical) molecules to be calculated before they are created, providing a significant cost savings to the Army. In addition, chemical sciences research may ultimately improve Soldier mobility and effectiveness through the development of light-weight and small power sources, renewable fuel sources, and new energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objective, and to maximize the impact of potential discoveries for the Army and the nation, the Chemical Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund research, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate materials for use in chemical and biological defense and to discover and design biomimetic molecular structures. The Chemical Sciences Division also coordinates efforts with the Materials Science Division to pursue the design and characterization of novel materials through new synthesis and processing methods, the evaluation of mechanical properties, and molecular-level studies of materials and material properties. Research in the chemical sciences also complements research initiatives in the Physics and Electronics Divisions to investigate the dynamics of chemical reactions and how chemical structures influence electrical, magnetic, and optical properties. The creation of new computational methods and models to better understand molecular structures and chemical reactions are also an area of shared interest between the Chemical Sciences and Mathematical Sciences Divisions. The research areas of the Chemical Sciences Division also overlap with research managed by the

Environmental Sciences Division, in which new methods and reactions are investigated for detecting, identifying, and neutralizing toxic materials. These interactions promote a synergy among ARO Divisions, providing a more effective mechanism for meeting the long-term needs of the Army.

B. Program Areas

To meet the long-term program goals described in the previous section, the Chemical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Polymer Chemistry, (ii) Reaction Dynamics, (ii) Electrochemistry, and (iv) Reactive Chemical Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Polymer Chemistry. The goal of this Program Area is to understand the molecular-level link between polymer architecture, functionality, composition, and macroscopic properties. The studies guided by this program may ultimately enable the design and synthesis of new polymeric materials that give the Soldier improved protective and sensing capabilities, and capabilities not yet imagined. This Program Area is divided into two research Thrusts: (i) Functionalized Morphology and (ii) New Synthetic Methodologies. Within these Thrusts, high-risk, high payoff research efforts are identified and supported to pursue the program's long-term goal. Research in the Functionalized Morphology Thrust is exploring how changes in molecular structure and composition impact macroscopic properties, to design polymer molecular architecture (*e.g.*, location of functional groups) to generate unique and well-defined morphologies, and to understand molecular-level, multicomponent transport in complex systems. Efforts in the New Synthetic Methodologies Thrust focus on developing new synthetic approaches for preparing novel polymers with potentially interesting properties, the design of new polymerizable monomers, and the design and synthesis of polymers with targeted responses.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include light-weight, flexible body armor, materials for clothing that are breathable but also provide protection from toxins, fuel cell membranes to harness renewable energy, and damage-sensing and self-healing materials for vehicles, aircraft, and other DoD materiel. In addition, the efforts promoted by this program may ultimately lead to new, dynamic materials such as photohealable polymers that can be used as a repairable lens coating and mechanically- or thermally-responsive polymers and composites that can convert external forces to predesigned internal chemical reactions (*i.e.*, to convert external force to internal self-repair).

2. Reaction Dynamics. The primary goal of this Program Area is to determine the pathways and intermediates for fast reactions of molecules in gas- and condensed-phases at high temperatures and pressures, and to develop theories which are capable of accurately describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program Area is divided into two research Thrusts: (i) Dynamics and (ii) Theory. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high-payoff research efforts that can collectively meet the program's overall goal. The Dynamics Thrust supports research efforts on the study of energy transfer mechanisms in molecular systems, while the Theory Thrust supports research to develop and validate theories for describing and predicting the properties of chemical reactions and molecular phenomena in gas and condensed phases.

The research efforts supported by this Program Area will likely enable many future applications for the Army and general public. These potential applications include more efficient and clean engine technology, the development of new tools to study condensed phases of matter, the capability to accurately predict the properties of theoretical molecules, and the development of novel molecules for use in energy storage.

3. Electrochemistry. The goal of this Program Area is to understand the basic science that controls reactant activation and electron transfer. These studies may provide the foundation for developing advanced power generation and storage technology. This Program Area is divided into two research Thrusts: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Redox Chemistry and Electrocatalysis Thrust supports research efforts to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those

surfaces, while the Transport of Electroactive Species Thrust identifies and supports research to uncover the mechanisms of transport through polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and to explore new methodologies and computational approaches to study the selective transport of species in charged environments.

The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications include the discovery and use of new mechanisms for the storage and release of ions that are potentially useful in future power sources, including new battery or bio-fuel concepts. In addition, studies of electroactive species may enable the development of multifunctional materials that simultaneously provide ionic conductivity, mechanical strength, and suitable electronic conductivity over a considerable temperature range, while exposed to aggressive chemical environments.

4. Reactive Chemical Systems. The goals of this program are to explore absorption, desorption, and the catalytic processes occurring at surfaces, and to investigate the structure and function of supramolecular assemblies (*i.e*, complexes of molecules held together by noncovalent bonds). Specific objectives include the discovery of new synthetic approaches to create self-assembled systems and the incorporation of catalytically or biologically active species into these systems. Through the study of these processes and structures, the program seeks to develop a molecular-level understanding of catalytic reactions, functionalized surfaces, and organized assemblies which could lead to future materials for protection and sensing. This Program Area is divided into two research Thrusts: (i) Surfaces and Catalysis and (ii) Organized Assemblies. Within these Thrusts, high-risk, high-payoff research efforts are identified and supported to pursue the program's long-term goals. The Surfaces and Catalysis Thrust supports research efforts on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces. Research efforts in the Organized Assemblies Thrust are exploring the properties and capabilities of self-assembled structures, including their functionality, and how to control assembly under different conditions.

This program supports research efforts that will likely lead to many long-term applications for the Army and the general public. These potential long-term applications include the development of stimuli-responsive materials for Soldier protection, the chemical sensing of hazardous materials, and the controlled release of reactive species for hazardous material destruction.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY10 were \$86.6 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) Program funding allotment for this Division was \$5.6 million. The DoD Multidisciplinary University Research Initiative (MURI) and Defense University Research Instrumentation Program (DURIP) provided \$6.5 million to programs managed by the Chemical Sciences Division. The Division also managed \$25.5 million of Defense Threat Reduction Agency (DTRA) programs, \$26.8 million of Defense Advanced Research Projects Agency (DARPA) programs, and \$4.4 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided \$9.9 million for awards in FY10. Congressional Earmarks provided \$6.7 million . Research funds in FY10 also included \$1.2 million provided through other sources for use in specific programs, including the Presidential Early Career Award for Scientists and Engineers (PECASE) program and the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) outreach program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. 18th Current Trends in Computational Chemistry Symposium (Jackson, MS; 30-31 October 2009). The 18th Conference on Current Trends in Computational Chemistry was a two-day conference held to discuss applications and the latest developments of computational chemical techniques for predicting properties of various chemical systems, including those of civilian and military importance. The conference covered both *ab initio* and semiempirical modeling, as well as *ab initio* molecular dynamics methods. Researchers from the Army Research Laboratory (ARL), the Engineer Research and Development Center (ERDC), the Army Corps of Engineers, and researchers from academia attended. Eleven invited speakers gave presentations and over 100 posters were presented. The conference topics included current progress in the development of computational methods and their applications in research. Among the topics presented were the application of computational methods for biological species, solvent effects, developments of density functional theory methods, environmental fate of nitrocompounds, kinetics of decomposition of explosives, and stability of chemical compounds.

2. Workshop on Roaming Dynamics and Multiple Mechanisms in Chemical Reactions (Argonne National Laboratory, IL; 18-20 April 2010). Combined experimental and theoretical work in recent years has provided unambiguous evidence of the existence of unconventional and overlooked reaction pathways in unimolecular decompositions and bimolecular reactions – pathways that involve near-decomposition of a closed shell molecule to radical products, followed instead by an intramolecular abstraction giving closed shell products. This "roaming" behavior, bypassing the nominal transition state, was first shown clearly in formaldehyde decomposition, although there was precedent in earlier work. This behavior is closely related to other examples of reactions that deviate significantly from the minimum-energy-path or that possess multiple pathways to the same products. This has clearly become a "hot topic" recently, and there is a growing consensus that it is a nearly universal phenomenon. However, the implications of these processes and pathways, both practical and theoretical, have not been fully explored. The goal of this workshop was to bring together experts in both theory and experiment, from academia and government laboratories, to explore the consequences of these newly recognized pathways in reaction kinetics, in combustion, in atmospheric chemistry, and in the theoretical description of reactive processes. One outcome of the workshop is that a general consensus was reached on research directions to pursue. One direction of interest to the Army is the possibility of roaming radical mechanisms which might come into play as an energetic material is shocked. Understanding of such phenomena can lead to the design of insensitive munitions.

3. ECBC Workshop – Surface Science and Interfacial Dynamics (Edgewood, MD; 9 December 2009). The purpose of this workshop was to introduce and solicit feedback from subject matter experts and performers on development of a Surface Science Center at ECBC. From this rapidly developing discipline emerge new scientific tools and approaches to materials synthesis, characterization, and modeling that can be used to understand agent interactions with coatings, porous catalysts, plants and animal cells, and in sensory recognition. A variety of leading researchers in the surface science field presented their work and views on how this multidisciplinary field has far reaching applications across the sciences. The development, organization, integration, research capabilities, and needs of a surface science center were also discussed. This has resulted in additional funding for this initiative.

4. Recent Advances at the Bio/Abio Interface Workshop (Christchurch, NZ; 22-24 June 2010). This multidisciplinary workshop brought together experts from academia and government laboratories to discuss recent advances in the area of bio/abio interfaces, including characterization tools at the liquid-solid interface, materials synthesis of biological/biologically inspired scaffolds, and molecular engineering of biological scaffolds. The work presented was applicable in a number of areas including materials, catalysis, electronics, medical devices, and drug delivery. During the course of the workshop, a variety of key challenges were identified that stimulated prospective research topics including understanding how dynamics play a role in self assembly and at interfaces, development of tools to study both orientation and environmental interactions at the interface, and development of mature simulation tools.

5. Chem/Bio Filtration Strategies Working Group (Arlington, VA; 31 August - 2 September 2010). The goal of this workshop was to develop strategies for the synthesis, development, and design of novel porous compounds, aerosol filtration media, and indicators for monitoring the residual life of next generation military filtration technologies. Both new and returning presenters from government and academia in the fields of aerosol filtration, adsorption science, catalysis, materials science, reaction kinetics, reticular chemistry, sensor development, and surface science were invited to participate in formal talks and discussions on building design rules and experimental evaluation techniques relevant to the filtration arena, and to develop strategies to optimize the performance of filtration systems against toxic industrial chemicals.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Chemical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Studying Molecular and Optical Properties of Nanophotonic Materials. This MURI began in FY06 and was awarded to a team led by Professor Eric Van Stryland at the University of Central Florida. This MURI is exploring the molecular structure of materials that display properties of high-speed nonlinear optics (NLO).

The field of NLO has enabled breakthrough developments in laser design, controlling light, and remote sensing. The goal of this MURI is to discover the structural components required for creating a new generation of materials that exhibit large NLO-absorption properties. If successful, this fundamental knowledge could be used in the future to create a new generation of nanophotonic materials that control light at or below nanometer wavelengths, which has the potential to revolutionize the telecommunications industry by providing high-speed interference-free devices on a microchip. In addition, these materials could lead to improved visible-imaging applications (*e.g.*, microscopy) and protective devices that will absorb high-energy light (*e.g.*, visors to protect the Soldier from sunlight or high-powered lasers, without interfering with visibility at dawn or dusk).

2. Investigating Mechanochemical Transduction. This MURI began in FY07 and was awarded to a team led by Professor Jeffrey Moore at the University of Illinois Urbana. This research is co-managed by the Chemical Sciences and Materials Science Divisions. This MURI is exploring mechanical-to-chemical energy conversion (*i.e.*, mechano-chemical transduction), including the design, synthesis, and characterization of a revolutionary new class of compounds that could potentially convert mechanical energy to catalyze chemical reactions.

The use of polymers and polymer composites in construction materials, microelectronic components, adhesives, and coatings is well established. Polymer composites can form strong materials for use in civil and government engineering, such as siding materials or armor. Unfortunately, these polymeric materials commonly crack when subjected to mechanical stress (damage), and these cracks can occur deep within the structure where detection is difficult and repair is almost impossible. These cracks are a visible manifestation of the chemical changes (*e.g.*, breaking of bonds) that occur at the molecular level when the structure is damaged. This MURI team is investigating the direct and reversible transduction between mechanical and chemical energy, and the potential to ultimately exploit this process in the design and synthesis of new materials. To meet this goal, the team of investigators is designing, synthesizing, and characterizing revolutionary new class of mechano-responsive molecules, called mechanophores, that are designed to respond to mechanical stress with pre-designed chemical reactions. Based on these results from this project, future molecules could be designed to convert mechanical stress (*e.g.*, structural damage) to useful chemical reactions. If this research is successful, applied research efforts in the future could use the results of this MURI to construct polymer composites that automatically alert the user to when and where a structure has sustained damage, and then self-repair after damage.

3. Molecular Design of Novel Fibers using Carbon Nonotubes. This MURI began in FY09 and was awarded to a team led by Professor Horacio Espinosa at Northwestern University. The focus of this MURI is to understand the molecular properties required for preparing strong fibers using polymers and double-walled carbon nanotubes (DWCNT).

The chief objectives of this research are to (i) develop a model system for predicting the molecular properties necessary for preparing new, high-strength fibers, and (ii) to prepare novel fibers composed of double-walled carbon nanotubes and polymers. The team will use multiscale computer simulations to bridge atomistic (*i.e.*, electronic structure methods and reactive force fields), coarse-grain, and continuum scales to explore and understand DWCNT-polymer interactions, crosslinking effects (bond-breaking mechanisms), and the impact of architecture on fiber strength, elasticity, and toughness. The investigators will use the results to predict fiber precursor properties necessary for optimum strength. The team will use predictive models to develop chemical vapor deposition techniques for producing highly-aligned DWCNT mats with optimized density and surface chemistry. The mats will serve as precursors for fiber formation. These materials will be characterized using *in situ* and *ex situ* microscopy (*i.e.*, assayed during and after reaction completion). The fundamental scientific knowledge uncovered through this research may lead to new approaches for designing and constructing high-strength, flexible fibers that are directly relevant to lighter-weight and flexible personnel armor.

4. Studying Ion Transport in Complex Organic Materials. This MURI began in FY10 and was awarded to a team led by Professor Andrew Herring at the Colorado School of Mines. This MURI team is investigating the interplay of chemical processes and membrane morphology in anion exchange.

Ion transport in complex organic materials is essential to many important energy conversion approaches. Unfortunately, ion transport is poorly understood in terms of its relationship to water content, morphology, and chemistry. While a great deal of research has focused on proton exchange membranes, little work has been performed with anion exchange membranes. This MURI team will study the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations will serve as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, the design and synthesis of robust, thin alkali-exchange membranes, combined with an improved understanding of ion exchange gained through the characterization of these membranes, could enable the development of new classes of fuel cells. If the MURI team can characterize the fundamental processes of ion exchange across these polymer membranes, future fuel cells using similar membranes could harness alkali exchange, resulting in inexpensive, durable, and flexible-source power for the Army and commercial use.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Low-power Nerve Agent Detector. Three Phase I CBD-SBIR contracts were awarded to Identizyme Defense Technologies, Inc., Luna Innovations, Inc., and Lynntech, Inc. to develop a nerve agent detection system that requires little to no operating power.

Chemical nerve agents pose a significant threat to the military and civilians. In the case of a hazardous material release, the exact identification of the active agent could enable faster and more effective medical and environmental responses. The ultimate goal of these SBIR projects is to develop an inexpensive, reliable, resilient, colorimetric sensor for detecting specific nerve agents. The goal of these projects in Phase I is to develop a fundamental understanding of the key recognition elements in various nerve agents, pesticides, and simulants. Using this knowledge, these groups will identify the technological requirements to develop sensors for accurately and selectively identifying a given agent. This type of detector could ultimately be used to identify a particular agent to which a warfighter or first-responder has been exposed, leading to the use of targeted measures for protection, decontamination, and treatment.

2. Dry Adhesive to Enhance Sealing of Respiratory Masks. A Phase II CBD-SBIR contract was awarded to Technova Corporation to optimize and test an adhesive for use in enhancing the sealing performance of a full-facepiece respiratory protective mask.

While man-made adhesives typically rely on chemical interactions, many biological species such as the gecko utilize a wide variety of mechanisms to attach and detach from surfaces. These mechanisms include elasticity, van der Waals forces (*i.e.,* attractive or repulsive intermolecular forces), structural design, and capillary forces. In combination with dry or oil-coated hairs, these biological adaptations enable strong, repeatable attachment and detachment, and are self-cleaning against dirt and any contaminants on surfaces. This SBIR builds on a Phase I effort, with the goal of developing fabrication techniques for incorporating a bio-mimetic adhesive (*i.e.*, mimicking properties found in biological systems) with the seals of a full-facepiece respirator. The adhesion properties of the mask with the adhesive incorporated will be assessed against unshaven, sweaty, and dirty skin, and in a variety of environments with varying temperature and humidity. Lastly, an optimized system will be fully examined through human subject testing. This research may ultimately benefit the Soldier by providing more reliable and flexible respiratory-protective devices.

3. Sensor for Monitoring Chemical Agent Exposure. A Phase II CBD-SBIR contract was awarded to Intelligent Automation, Inc. to develop and validate a prototype real-time sensing system for the detection of a simulated chemical agent, methyl salicylate (MeS).

Recent advances in detection technologies and semiconductor development may allow the development of systems that can more accurately and selectively detect chemical vapors in trace quantities. This project continues efforts initiated in a Phase I effort, with the goal extended to developing and validating a prototype MeS sensor system for real-time detection of MeS infiltration through a protective garment. The prototype will be tested to ensure functionality when fitted near a number of body regions, in the presence of human sweat, in varying temperatures, and in rapidly-fluctuating air flow. A MeS sensor system could provide data throughout the duration of a simulated chemical exposure or if simulated leaks should occur in protective clothing while worn by active military personnel. These data can be used to develop improved protection methods for Soldiers as well as predict the battlefield conditions where Soldiers may require greater protection.

4. Electrochemical System for On-demand Chemical and Biological Decontamination. A Phase III CBD-SBIR contract was awarded to TDA Research, Inc. to develop a novel liquid solution for chemical and biological decontamination based on electrochemical technology.

Detergents and other surfactants are commonly used to remove chemical and biological agents from surfaces. However, a common problem in decontamination is how to provide a formulation that is stable for years in an inactive form and can be activated on demand to produce a very reactive cleaning solution that does not remain active in the environment. This CBD-SBIR project seeks to develop and test an advanced surfactant formulation and delivery system for the removal of chemical and biological agents. This Phase III effort will build on results from earlier phases to further develop a delivery approach that employs an electrolytic cell to activate a chemical species that can then break down chemical or biological warfare agents. The product candidates will be tested with a variety of spray applicators, in multiple environments, and against a variety of chemical and biological targets. The goal is to optimize the surfactant formulation, producing a species that is stable in storage, but that can be released on demand exactly when and where it is needed. The optimized formulation will be highly

reactive and thus capable of quickly cleaning a surface, but then degrade quickly and not persist in the environment. This system, if successful, could be used by the U.S. military and first responders for immediate bio-decontamination of vehicles or equipment contaminated with bio-warfare or chemical warfare agents (CWAs).

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Nanoparticle-mediated Decontamination of Toxins within Forensic Containers. Two Phase I STTR projects were funded with Materials Modification, Inc. and Nanoscale Materials, Inc., to develop a textile liner composed of metal oxides that enables the absorption and decontamination of chemical and biological warfare agents within a forensic storage container. The storage, transport, and analysis of materials contaminated by chemical or biological warfare agents is complicated by the fact that many currently-available storage containers can degrade, potentially leading to secondary exposure of the toxic chemicals. These Phase I STTR projects are developing, characterizing, and testing metal oxide nanoparticle sorbents for use in a liner for forensic containers. To pursue this goal candidate compounds will be characterized for their efficacies in breaking down various CWA stimulants and for antimicrobial activity against *E. coli* or other species. In addition, these efforts will investigate methods for integrating the metal oxides into fabrics. Using the results from these studies, the investigators will develop fabric liners for forensic containers that can meet Army needs in hazard mitigation and Soldier protection. In addition, this technology could potentially be extended to other applications such as chemotherapy-drug decontamination and disposal, air/water filtration, elimination of antimicrobial products, and protection against toxic industrial chemicals.

2. Activated Reactants to Improve Fuel Cell Power Density. Two Phase I STTR contracts were awarded to Entroplus Technology Solutions and Services, LLC and JSJ Technologies, LLC to develop new methods for increasing the power density of fuel cells.

A long-standing Army need is to develop lower-weight, reliable power sources. Fuel cells convert a source fuel into electrical power. They are similar to batteries in that they are both electrochemical devices; however, fuel cells do not require recharging and can produce electrical power as long as sufficient source fuel is available. The electric current produced by a fuel cell is primarily dependent on the rate of the electrode reactions. A variety of methods have been explored for driving the electrode reactions (*e.g.*, adding heat or lowering the required activation energy of the reactants); however, these approaches have been met with limited success. These STTR projects are investigating and developing new methods to chemically activate some or all of the fuel cell reactants, thereby increasing the rate of the electrode reactions. The candidate methods will be tested and optimized to provide the greatest improvement to the overall power density of a fuel cell, while minimizing the additional supporting hardware required to activate the reactants. If successful, these methods for activating reactants in fuel cells could provide a mechanism for reducing fuel cell size and weight at a given power level, which is relevant to future Army needs in mobility and efficiency.

3. Catalytic Membrane Reactor for Renewable Hydrogen Production. Two Phase I STTR contracts were awarded to FuelCell Energy, Inc. and InnovaTek, Inc. to develop a fuel processor system capable of producing hydrogen from butanol.

Due to their reliably long duration of performance, batteries are used to power most portable military and commercial electronic devices. The batteries are typically produced and recharged using power from non-renewable energy sources, and the batteries pose an environmental hazard if not properly discarded. These Phase I STTR projects are developing methods for catalyzing the production of hydrogen from butanol for use in a proton exchange membrane (PEM) fuel cell. Various catalysts will be designed, tested, and optimized for capabilities in oxidizing butanol to release hydrogen. The effectiveness of the optimized catalyst in powering a PEM fuel cell will then be assessed, and if successful, these efforts may lead to a fuel cell system that can be recharged using butanol, a renewable energy source. This system would provide the U.S. military and civilians a more environmentally friendly, portable, and renewable power source relative to batteries or traditional internal-combustion engines.

4. Novel Rapid and Reliable Testing Methodologies to Assess Fuel Quality. Two Phase I STTR projects were funded with Engineering and Scientific Innovations, Inc. and InnoSense, LLC to develop a new method for rapidly and reliably testing the quality of fuels produced when compared to the Jet Propellant 8 (JP-8) standard.

Army vehicles and aircraft require fuel of sufficient quality to prevent damage to materiel or injury to personnel. The currently available tests for measuring the smoke point and thermal stability of JP-8 fuels are subject to significant operator judgment and potential bias. Each of these STTR projects will design and characterize novel, candidate methods for measuring the thermal stability or the smoke point of JP-8 fuels, and then optimize a single method capable of rapidly and reliably making these measurements, while requiring little or no operator judgment and only a minimal amount of fuel for testing. If successful, the technologies developed under these agreements could have a significant impact on military and civilian fuel distribution, testing, and quality control, as well as providing a potential tool for the aviation, refining, and pipeline industries.

5. Ceramic Electrolytes for Next-generation Lithium-air Battery. A Phase II STTR agreement was established with CHEMAT Technology, Inc. to develop a lithium-ion conducting ceramic electrolyte incorporated into a lithium-air battery.

Lithium-ion batteries have a high energy density, and their low weight makes them more practical for use in electric cars and portable power sources relative to the older nickel-cadmium or lead-acid batteries. Despite their high energy density, lithium-ion batteries have a relatively low power density. This Phase II STTR project seeks to incorporate the lithium-ion conducting ceramic electrolyte developed in Phase I into a lithium-air battery pack, and then assess its energy and power capacity. The electrochemical characteristics of the lithium-air system will be assessed, as will the chemical and electrochemical stability of the battery. A successful and marketable lithium-air battery will contribute to military and civilian applications, including portable optics, sensors, and communications equipment.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Characterizing Interactions of Carbon-based Materials and Toxic Materials. A new HBCU/MI award was granted to Professor Teresa Bandosz at the City University of New York to investigate the fundamental interactions and reactive properties of nano-engineered carbon-based materials with toxic industrial chemicals.

Graphite oxides, metallic organic frameworks (MOFs), and related compounds have been shown to be capable of removing trace amounts of small molecule gases, such as toxic industrial compounds. However, the mechanism through which these compounds reactively absorb gases under ambient conditions is not well understood. Through this HBCU/MI research project, the investigator will synthesize a variety of carbon-based composites, including graphite MOFs and activated carbon composites. The structures, surface chemistry, and relative rates of gas adsorption of these materials will be experimentally determined. The results of these studies will provide a fundamental understanding of the mechanism of reactive adsorption of various molecules on carbon-based nanocomposite materials. This research will also provide data for use in the future synthesis of new, optimized MOFs or other materials which have potential applications in the decontamination of CWAs or toxic industrial compounds.

2. Investigating Hydrocarbon Decomposition Using Aerogel-based Catalysts. A new HBCU/MI award was granted to Professor Jale Akyurtlu at Hampton University to study hydrocarbon reformation using novel aerogel-supporting catalysts.

All branches of the armed services have high energy requirements. As in the private sector, this energy is often produced by the non-renewable combustion of hydrocarbon fuel. The Army and DoD seek to improve the energy efficiency of U.S. forces in part by switching to hydrogen as an energy carrier. Hydrogen fuel cells can provide electrical power from a hydrogen fuel source. The chemical mechanisms for the production of hydrogen from renewable fuel sources are poorly understood. This research is exploring the mechanisms of hydrocarbon

reformation—a process that can provide a renewable energy source by using chemical catalysts to form hydrocarbons from water and carbon dioxide. The investigator will design metal-containing aerogels for subsequent use as catalysts in hydrocarbon reformation. Aerogels are derived from gels, but have the liquid component removed. These unique structures have an extremely high surface area and high potential reactivity. The activity and selectivity of the various aerogel catalysts in forming hydrocarbon products will be measured, and the mechanisms of each reaction approach will be characterized. This study will provide a greater understanding of potential catalysts and mechanisms for use in hydrocarbon reformation. The results of this project may enable the development of highly active and stable fuel-reforming catalysts for renewable hydrogen production.

3. Infrastructure for New Science Laboratory. A TCU award was granted to Professor John Rombold at Northwest Indian College for the purchase of equipment to outfit a new research laboratory. The Northwest Indian College expects to build a new research laboratory (supported from other grants); however, the existing funds will not cover the cost of the basic infrastructure for the new facility. This TCU award will enable the school to purchase equipment for undergraduate and graduate students to pursue research and experimentation in the areas of environmental chemistry, inorganic chemistry, and marine biology, among others.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Chemical Sciences Division managed eleven new DURIP projects, totaling $1.2M. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of electrocatalysts, the thermal properties of polymers, and the gas-phase decomposition of energetic materials.

I. University Affiliated Research Center (UARC): Institute for Soldier Nanotechnologies (ISN)

The ISN, located at the Massachusetts Institute of Technology, carries out fundamental, multidisciplinary, nanoscience research that is relevant to the Soldier. Nanoscience research creates opportunities for new materials, properties, and phenomena as material properties (*e.g.*, color, strength, conductivity) become size dependent below a critical length scale of about 500 nanometers. The research performed at the ISN falls into five Strategic Research Areas (SRAs): (i) Light Weight, Multifunctional Nanostructured Fibers and Materials, (ii) Battle Suit Medicine, (iii) Blast and Ballistic Protection, (iv) Chemical and Biological Sensing, and (v) Nanosystems Integration. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the ISN program website (http://mit.edu/isn/research/index.html).

The ISN currently supports 45 faculty, 100 graduate students, and 40 postdoctoral fellows across 12 departments at MIT. The ISN program is unique in that it currently has 14 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ISN research portfolio, assessing the goals of the various projects and research results. The ISN and its industry partners are well-situated to perform basic and applied research in response to Soldier needs now and in the future. A total of $9.4M was allocated to the ISN for 6.1 basic research in FY10, and $3.2M was awarded for eight 6.2 level projects including three new projects.

J. Joint Science and Technology Office for Chemical and Biological Defense

Traditionally ARO has been a strong partner with the Chemical Biological Defense (CBD) Program. The Reactive Chemical Systems Program manages several basic and applied research efforts for the CBD program. The goal of this program is to develop technologies for protection of the warfighter from chemical and biological agents. Basic research efforts in the areas of biomimetic catalysts, bio/abio interfaces, and mass transport and diffusion are aligned with and enhance the Army basic research program. Research in this program includes fundamental surface chemistry, molecular recognition, and enzyme stabilization. ARO also manages the Decon Enabling Sciences program which strives to accelerate the transition of fundamental research to the development of decontamination and chemical detection technologies.

K. DARPA Biofuels Alternative Feedstocks

The Biofuels Alternative Feedstocks program is developing affordable alternatives to petroleum-derived JP-8, instead using algae and cellulosic biomass. DARPA seeks to develop and demonstrate the technology that can enable the production of JP-8 at less than $3 per gallon at a moderate-scale facility (<50 Mgal/yr) and that can be broadly and repetitively implemented to have pervasive impact on the DoD. The Electrochemistry and Electrocatalysis Program manages this effort on behalf of DARPA.

L. DARPA Limits of Thermodynamic Storage of Energy

DARPA is soliciting innovative proposals to develop revolutionary new approaches to portable energy sources. DoD is critically dependent on portable electronics and, by extension, portable energy sources such as batteries. However, the actual energy output of state-of-the-art battery technologies, such as the BA5590 $LiSO_2$ primary and BB2590 Li-ion secondary systems, fall short of their projected energy capacity under load, limiting the operation of DoD electronic systems using these batteries to as little as 20% of theoretical capability. This operational inefficiency increases the number of batteries Soldiers must carry in the field and also limits implementation of hybridization and distributed power concepts for DoD ground, aerial, and maritime vehicle platforms. The DARPA Limits Of Thermodynamic Storage (LOTS) of Energy program seeks to address inefficiencies in energy extraction by developing technologies that are capable of delivering the full expected run time out of a state-of-the-art portable energy source. This DARPA program is managed through the Division's Electrochemistry and Electrocatalysis Program.

M. Fuel-cell Based Squad Battery Charger Quick Reaction Fund

Current military operations rely heavily on batteries to power portable equipment. Providing batteries to the individual Soldier has become a major logistical challenge to the modern Army. While significant progress has been made in developing alternate power supplies, including prototype individual fuel cells, batteries are expected to remain the primary power source for the individual Soldier for the foreseeable future. If quiet, compact, lightweight and energy-dense chargers were available in sizes appropriate for small-unit operations, then Soldiers could continue using batteries, but reduce their weight burden by a factor of two or more by replacing primary batteries with rechargeable batteries and a high-efficiency battery charger operating on liquid fuels. To address the need for portable battery chargers sized for small squad operation, Protonex Technology Corporation is developing a prototype 125W portable generator based on solid oxide fuel cells. This generator uses low-sulfur kerosene as a fuel and is capable of operating both as a battery charger or directly powering equipment. With a mass of <7 kg, the battery charger would fit within a backpack. Using high energy-density kerosene fuel, the charger-based system could save more than 60% of the weight of current solutions. When used to power equipment directly, the fuel cell system saves more than 80% of the weight of the primary batteries. Within this program Protonex built and delivered prototype systems to both the Army and Navy for testing and evaluation. This Quick Reaction Fund Program is managed through the Chemical Sciences Division, Electrochemistry and Electrocatalysis Program and is coordinated with the ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Communications-Electronics Research, Development, and Engineering Center (CERDEC), and ONR.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Chemical Sciences Division.

A. New Approach to Calculations of Intermolecular Forces between Large Energetic Molecules

Professor Krzysztof Szalewicz, University of Delaware, Single Investigator Award

The objective of this research is to develop density functional theory (DFT) that accurately and efficiently calculates the intermolecular potential energy of a wide range of condensed-phase systems. While DFT is a good choice for carrying out electronic structure calculations for large systems, current DFT methods poorly describe dispersion. An improved DFT method that accounts for dispersion could allow for more accurate studies and predictions of reactions involving energetic compounds.

Professor Szalewicz is developing the local, linearly-scaling dispersion component of symmetry adapted perturbation theory based on DFT of monomers [SAPT(DFT)]. This component contains two computationally intensive stages: calculation of the frequency-dependent density susceptibilities (FDDS) of the monomers (related to dynamic polarizabilities) and contraction of the FDDS's with two-electron integrals to evaluate the dispersion energy. When sparsity (*i.e.*, cases in which matrix elements of values near zero are not evaluated) is utilized, such calculations scale linearly and are thus highly desirable when compared to *ab initio* calculations which scale to the fifth power or higher in the number of basis functions (*i.e.*, *ab initio* calculations relying on first-principles that have higher demands on computational power).

For the prediction of intermolecular properties, like crystal structures, it is important to have an accurate description of dispersion. Professor Szalewicz has been pursuing the development of a dispersionless density functional theory (dlDFT). dlDFT takes advantage of the fact that the supermolecular DFT calculations can provide reasonable estimates of all components of the interaction energy except the dispersion energy. Dispersion can then be added back into the system later, resulting in a method known as dlDFT + D. This year, a dlDFT was successfully developed by optimizing the DFT parameters based on the Perdew–Burke–Ernzerhof exchange-correlation functional and the local-density approximation correlation functional, to reproduce dispersionless interaction energies of a training set. The continuing research effort concentrates on optimizing a form of dlDFT that can be applied without specifying any monomers. An example application of the dlDFT + D method, using the HMX dimer, a model energetic compound, is shown in FIGURE 1.

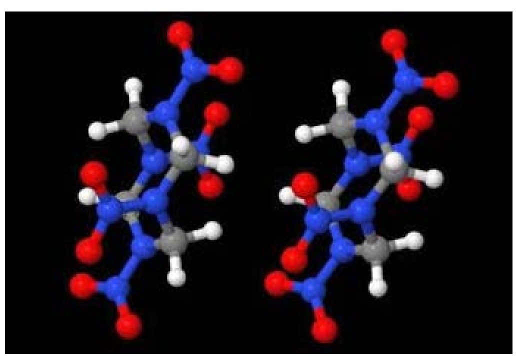

FIGURE 1

Minimum-energy geometry of the HMX dimer. This dimer (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocane) is an energetic system containing 56 atoms, calculated using a dlDFT + D method developed in the Szalewicz research group. Such results can be used to predict the crystal structure of the pure bulk compound.

The development of these theoretical models will allow for high accuracy computation of the reaction pathways and energies for the detonation of energetic materials, and for predicting the crystal structure of the solid forms of newly-developed energetic materials. In the dlDFT method, the dispersion component is subtracted and then added back later from another, more accurate method for calculation of dispersion. This method could allow the calculation of intermolecular potentials for large molecules with as many as 200 atoms.

B. Quantum Chemical Methods to Study Structure, Spectra, and Reaction Paths of Energetic Molecules
Professor Rodney Bartlett, University of Florida, Single Investigator Award

The goal of this research is to develop new, efficient computational algorithms for massively parallel implementation of the coupled cluster (CC) *ab initio* method. CC methods also allow for modeling of excited state potential energy surfaces which are important when state hopping occurs, such as when electronic relaxation through a conical intersection occurs, or for photochemical processes. Ultimately, this method will allow for quantitative predictions of chemical reaction phenomena, such as rate constants, through the generation of accurate potential energy surfaces for chemical reactions, plus their transition states and associated activation barriers. These CC methods do not depend on any empirical parameters, thus their application to the initial steps in the description of chemical processes that occur during detonation of energetic molecules and materials will be critically important in understanding such phenomena. The investigator is pursuing a dual-pronged approach to develop new, CC quantum chemical methods that will provide more accurate results than are available today.

The most popular implementation of CC theory includes single and double excitations (CCSD) with non-iterative triple contribution CCSD(T). The full inclusion of the T_3 operator method (triple excitations) has been used for high accuracy calculations of ground electronic states near stationary points. For studies involving higher accuracy, quadruple excitations are required. Bartlett introduced the T_4 cluster in its lowest-order perturbative contributions (fifth-order in the energy). The resulting CCSDTQ-1 method was shown to be an improvement over the CCSDT method, however it is costly since it scales as the ninth power in the number of basis functions (*i.e.*, it is so computationally expensive that it is impractical to use). Subsequently, the Bartlett group developed an alternative method that replaced the non-iterative term with a factorized formula that reduced the rank of the computational procedure to seventh order. This approach enabled computations using relatively large basis sets, which is important for high accuracy.

In the spirit of the goals of this research, even more efficient and accurate CC computational algorithms are being sought. In the current work, the Bartlett group developed the ΛCCSD(TQ_f) method, in which triple excitations and fifth-order factorized connected quadruple excitation operators are included in the CC wave function based on the Λ functional in a non-iterative way. This method has n^7 scaling and good convergence properties for equilibrium geometries and also for distorted geometries (*i.e.*, this method enables fast calculation of the CC wavefunction through the quadruple substitution level using a minimal amount of computer memory). Test applications for bond stretching of the diatomic molecules HF and N_2 are presented in FIGURE 2.

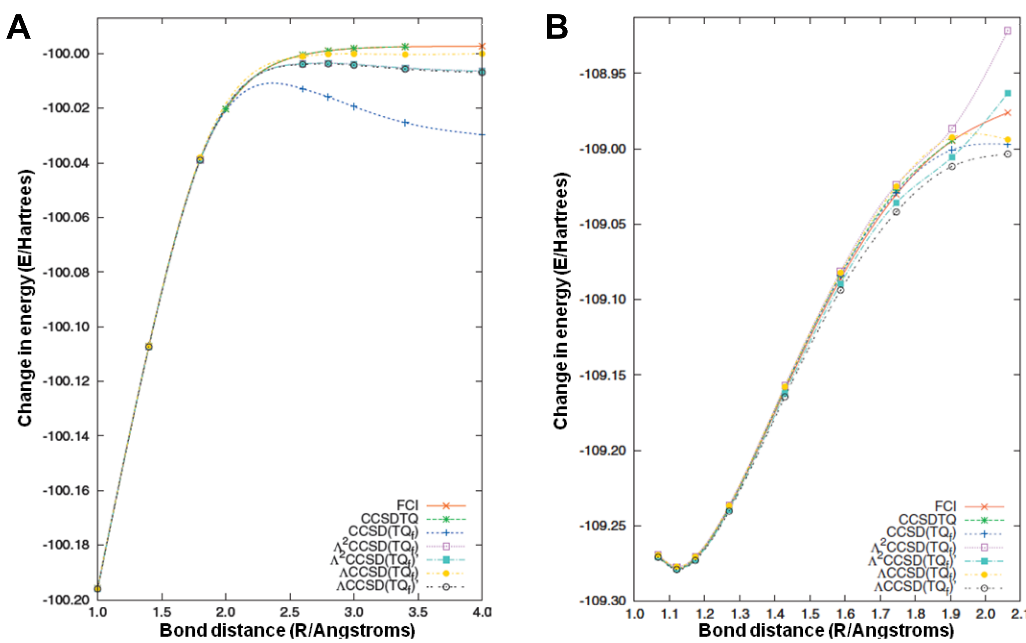

FIGURE 2

Potential energy curves for HF and N_2 molecules. The CC method was used to calculate the change in energy (y axis) as the bond distance of the molecule (x axis) increased for the (**A**) HF and (**B**) N2 molecules. For comparison, the FCI result is exact within the limited space defined by the basis set.

Due to incorrect separation for homolytic bond cleavage, RHF-based studies of potential energy surfaces continue to offer an extreme test for the validity of such CC variants. The full configuration interaction (FCI) method represents the exact solution of Schrodinger's equation within the limit of the finite basis set; hence it is the reference method. For the HF molecule, the ΛCCSD(TQ_f) method gives a good approximation to the FCI result at H-F distances in the bond-breaking region of 2.5 to 4.0 Ångstroms (see FIGURE 2A), while the N_2 molecule, with its triple bond, offers an even more challenging test of the theory (see FIGURE 2B). The reference method is FCI. For this molecule, all CC methods begin to deviate significantly at an N-N distance of 2.0 Ångstroms. Future work will explore the properties of energetic compounds using these methods, including bond dissociation energy pathways for homolytic dissociation.

Preliminary results showing the relative energies of various conformers of the RDX molecule, calculated using CC theory, are illustrated in FIGURE 3. Given that the RDX molecule exists in several conformations that are closely spaced in energy, all of these conformers and their relative energies are relevant to understanding the detailed spectra and structure of RDX.

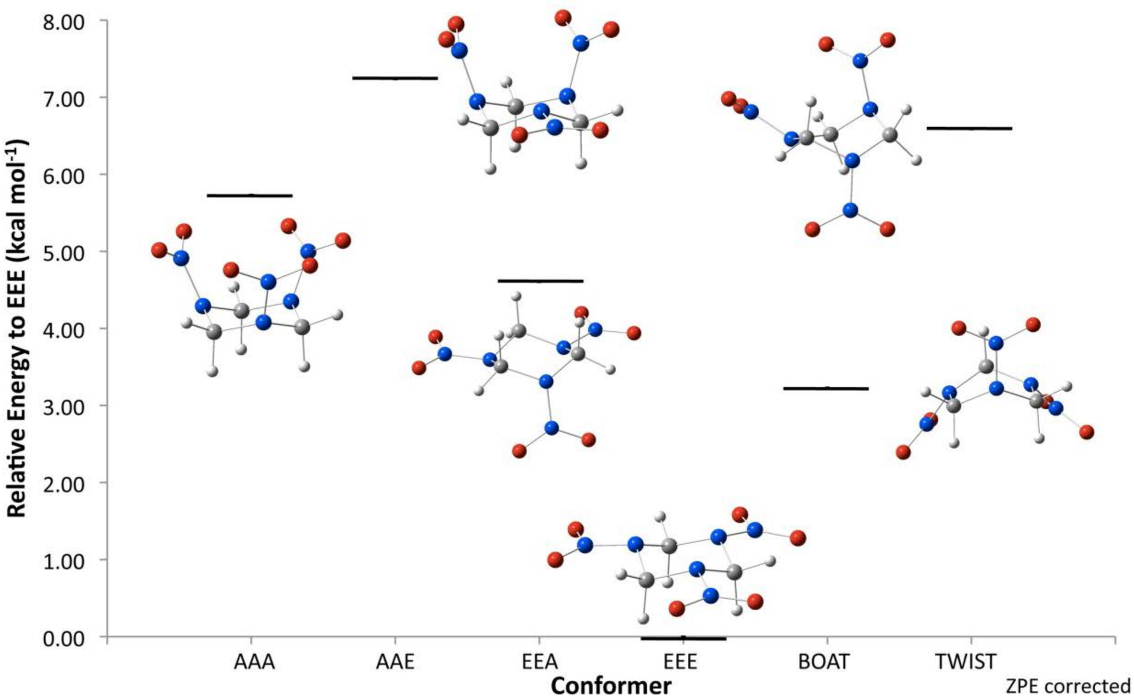

FIGURE 3

Relative energies of RDX conformers. The energies (y-axis) of RDX conformers (x-axis), relative to the lowest energy form (EEE) were calculated using the CC method developed by the Bartlett laboratory.

C. Probing Nanoparticle Reactivity at the Single-molecule Level

Professor Peng Chen, Cornell University, Single Investigator Award

Professor Chen has developed a single-molecule fluorescence approach to study metal nanoparticle catalysis at single-particle, single-turnover resolution in real time and under ambient solution conditions. The catalytic reduction of resazurin to resorufin by NH_2OH on a single Au-nanoparticle can be precisely monitored by the fluorescence turnover trajectories (see FIGURE 4). The sharp increases in fluorescence intensity indicate product formation on the nanoparticle surface, while the decrease in intensity represents product dissociation from the nanoparticles. Each off-on cycle corresponds to a single turnover of catalytic product formation on a nanoparticle and subsequent dissociation.

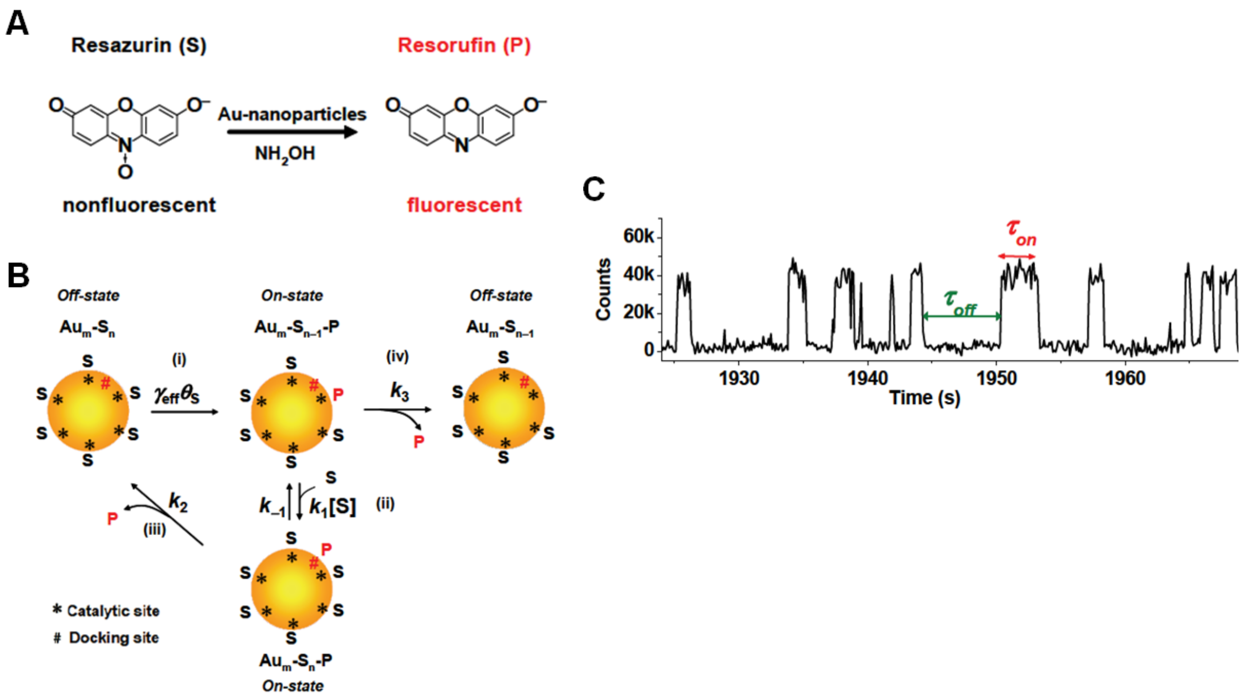

FIGURE 4

The catalytic reduction of resazurin to resorufin by NH_2OH on an Au-nanoparticle. (A) Au-nanoparticle catalyzed reduction of resazurin to resorufin. (B) Kinetic mechanism of nanoparticles-induced catalysis of the resazurin-resorufin reaction. (C) Fluorescence turnover trajectory of a single Au-nanoparticle.

Professor Chen has studied the effect of nanoparticle size on catalytic activity and selectivity. By monitoring the catalysis of 6.0, 9.1, and 13.7-nm (diameter) nanoparticles, it has been observed that smaller particle size correlates to decreased substrate binding affinity and an increase in catalysis, while product binding affinity increases with decreasing particle size. Two parallel product dissociation pathways exist, and larger nanoparticles appear to be less selective between the two pathways. This single-molecule fluorescence approach can be used to investigate the destruction of CWAs. Initial experiments with the fluorogenic oxidation of an acetyl dihydroxyphenoxazine derivative illustrate C-N bond cleavage, a critical step in CWA destruction.

D. Nanoscale Probing of Electrical Signals in Biological Systems

Professor Mark Hersam, Northwestern University, PECASE Award

This research effort focuses on development of conductive atomic force microscopy (cAFM) techniques that can spatially map the location of trans-membrane ion channels with nanometer-scale spatial resolution in the native physiological buffer solution of living cells. Scanning ion conductance microscopy (SICM) has become a useful tool for imaging biophysical systems. It can be integrated with other techniques such as confocal microscopy, scanning near-field optical microscopy, and patch clamping in order to obtain complementary information that correlates with the surface topography obtained from SICM imaging. However, SICM is insensitive to electrochemical properties, which play an important role in biological systems. In addition, scanning electrochemical microscopy can be used for spatial mapping of electrochemistry.

Professor Hersam has merged these tools together and successfully fabricated and demonstrated a nano-pipet probe (used with SICM) with an integrated ultra-microelectrode (used for SECM) for concurrent SICM and SECM imaging (see FIGURE 5).

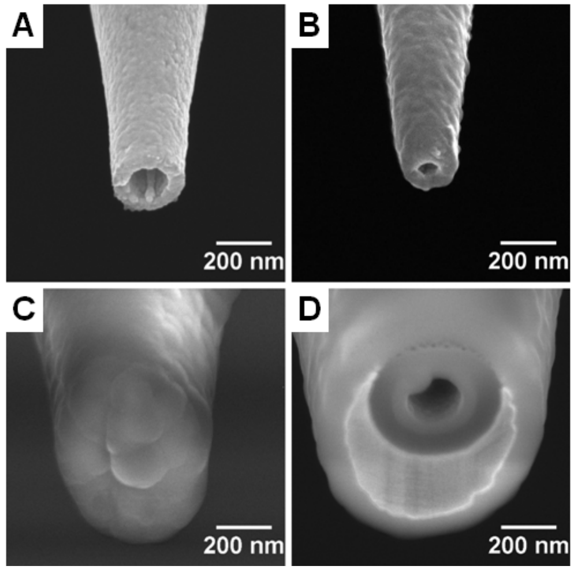

FIGURE 5

SEM images of SECM-SICM nanopipette throughout the fabrication process. (A) As-pulled borosilicate nanopipet with 30 nm AuPd film to minimize charging, (B) After evaporation of the gold electrode film with titanium adhesion layer, (C) After ALD of 100 nm thick Al_2O_3 with occluded nanopipet tip, and (D) After FIB milling to expose the gold and open the nanopipet tip.

Integrated SECM-SICM imaging was demonstrated in both feedback-mode and substrate generation/tip collection-mode imaging on patterned surfaces. The probe allowed for successful SECM-SICM imaging on features as small as 180 nm in size. This was demonstrated on FIB-patterned test structures consisting of arrays of narrow trenches FIB-milled into a gold film on a glass substrate (see FIGURE 6).

An improved molecular-level description of trans-membrane ion channels has the potential to impact many areas of military and civilian importance such as disease diagnosis, drug development and screening, and technologies that interface between living cells and microelecetronic circuitry.

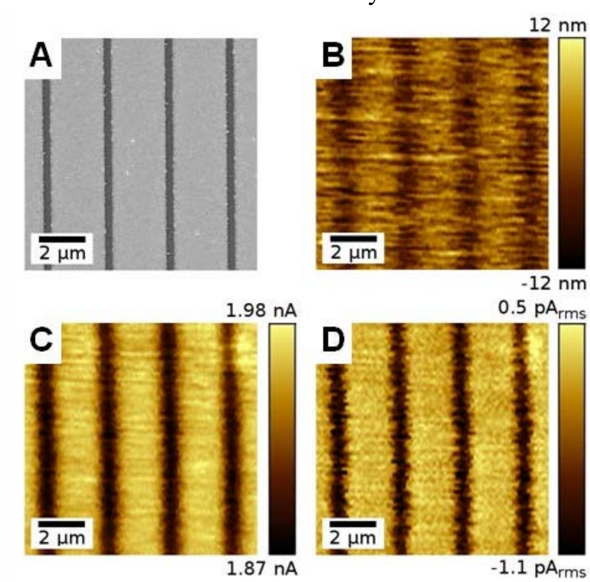

FIGURE 6

SEM and SECM-SICM images of 400 nm wide trenches FIB-milled into a gold film on a glass substrate. (A) SEM; (B) SECM-SICM topography; (C) SECM-SICM DC redox current; (D) SECM-SICM AC redox current.

E. Principles for Interfacial Engineering and Superstabilization of Biphase Systems Using Particles with Engineered Structure and Properties

Professor Orlin Velev, North Carolina State University, Single Investigator Award

Professor Velev is leading a research effort on designing interfacially-active particles that can afford unique properties and features to films, foams, and emulsions such as stability, color, and specific rheological response. The fundamental physical and chemical properties responsible for the interfacial activity are being studied.

This research led to the discovery of novel particle stabilizers for pickering foams and emulsions that can be modified either with dye to produce colored foams, or magnetic particles to produce magnetically-responsive foams. Magnetically-responsive foams were made using iron particles functionalized with oleic acid, combined with pH specific, hydrophobically modified, cellulose solution (HP55) stock (see FIGURE 7).

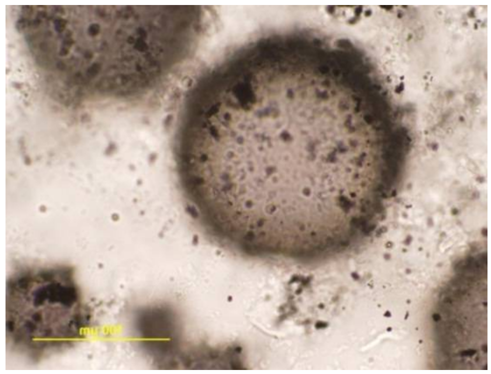

FIGURE 7

Optical micrograph of magneto-pickering foam. The HP55 stock (larger spheres) and functionalized iron particles (small black dots) are visible.

These foams were found to be stable for more than a week, but can be collapsed immediately upon application of a magnetic field. The foam breakdown time and collapsed foam volume was determined to be age and magnetic-particle-concentration dependent. In contrast, older foams contain less water and thus are less elastic leading to faster collapse (see FIGURE 8). Magnetically-responsive foams can potentially be used in general cleaning applications, leaving a low environmental footprint, as well as for use in the adsorption, removal, and destruction of hazardous materials.

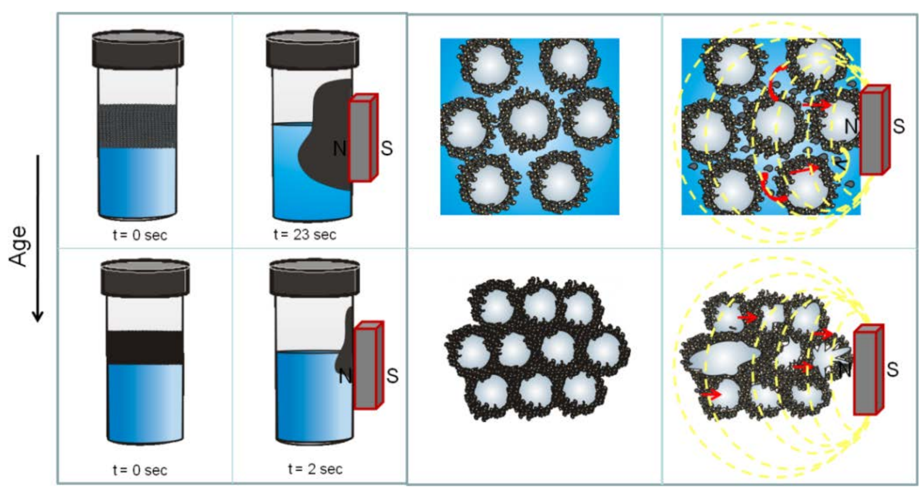

FIGURE 8

Proposed mechanism of foam collapse as a function of age. While older foams (bottom row), complete collapse within 2 seconds of applying the magnetic field, new foams (top row) do not complete collapse even after 23 seconds of applying the magnetic field.

F. Precision Morphology in Sulfonic, Phosphonic, Boronic, and Carboxylic Acid Polyolefins

Professor Kenneth Wagener, University of Florida, Gainesville, Single Investigator Award

This research focuses on the synthesis of polymers possessing ionic liquid entities. While the synthesis of such polymers has been challenging, this investigator published the first synthesis of polymers of this type, which show remarkable physical properties (Aitken, *et al.,* 2010). The polymerization was initiated in a small glass reactor under bulk conditions and the viscosity of the polymer increased so quickly that the polymerization resulted in breakage of the glass reactor. It is believed this is a result of either stress-induced crystallization of the polymer, or more likely, shear thickening that occurs upon the application of stress. The film can be slowly stretched, but rapid application of stress results in a quick "hardening" of the material loss of all elasticity (see FIGURE 9). As the morphology and physical characteristics of the polymer are not yet characterized, the research continues with the goal of producing several versions of the polymers for further characterization.

FIGURE 9

Film of polyolefin polymers prepared using ionic liquids. The film can be slowly stretched; however, rapid application of stress results in a quick "hardening" of the material and it loses all elasticity.

G. Photo-healable Supramolecular Polymers

Professor Stuart Rowan and Professor Christoph Weder, Case Western Reserve University, Single Investigator Award

Through an ARO Single Investigator award, Professor Stuart Rowan and Professor Christoph Weder are exploring chemical mechanisms for the photo-induced repair of polymers. This research recently led to the development of a family of metallosupramolecular polymers in which mechanical damage is efficiently healed upon exposure to light. These materials were made by the supramolecular polymerization of a ditopic macromonomer comprised of a 2,6-bis(1'-methylbenzimidazolyl)pyridine ligand end-capped with poly(ethylene butylene), with zinc and lanthanum salts (see FIGURE 10A). When the polymers were exposed to ultraviolet radiation, the metal-ligand motifs are electronically excited and the absorbed energy was converted into heat. This caused temporary disengagement of the metal-ligand motifs, concomitant with a reversible decrease of the viscosity. As a result, defects can heal quickly and with high efficiency upon exposure to ultraviolet light (see FIGURE 10B). Since light can be applied locally to the damage site, objects can be healed under load (see FIGURE 10C) and the reversible binding scheme allows for repeated healing. The researchers are continuing to study photo-induced repair to determine its dependence on factors such as polymer composition, polymer entanglements, and the metal salts and ligands that are responsible for the supramolecular assembly of the ditopic macromonomers.

The concept of photo-thermal induced healing of supramolecular materials is potentially applicable to any supramolecular polymer comprised of a suitable chromophore and a binding motif that is sufficiently dynamic. The ability to systematically change the chromophore allows one to tailor the wavelength and intensity of the light required for healing. The combination of this new approach with an additional mechanochromic response may enable autonomously self-healing materials, in which light is only absorbed at defect sites. It is possible

that such materials will have significant impact in protective coating applications. For example, materials or coatings that can be healed will dramatically increase the durability of a device, vehicle or structure. Such an increase in lifetime and durability is particularly import in the battlefield where replacement parts may not be easily accessible. The continuing trend to employ semi-autonomous and autonomous robots in the battlefield would benefit from new structural materials and coatings that can either heal themselves or that can be easily healed upon exposure to a readily available stimulus and without the need for labor-intensive intervention.

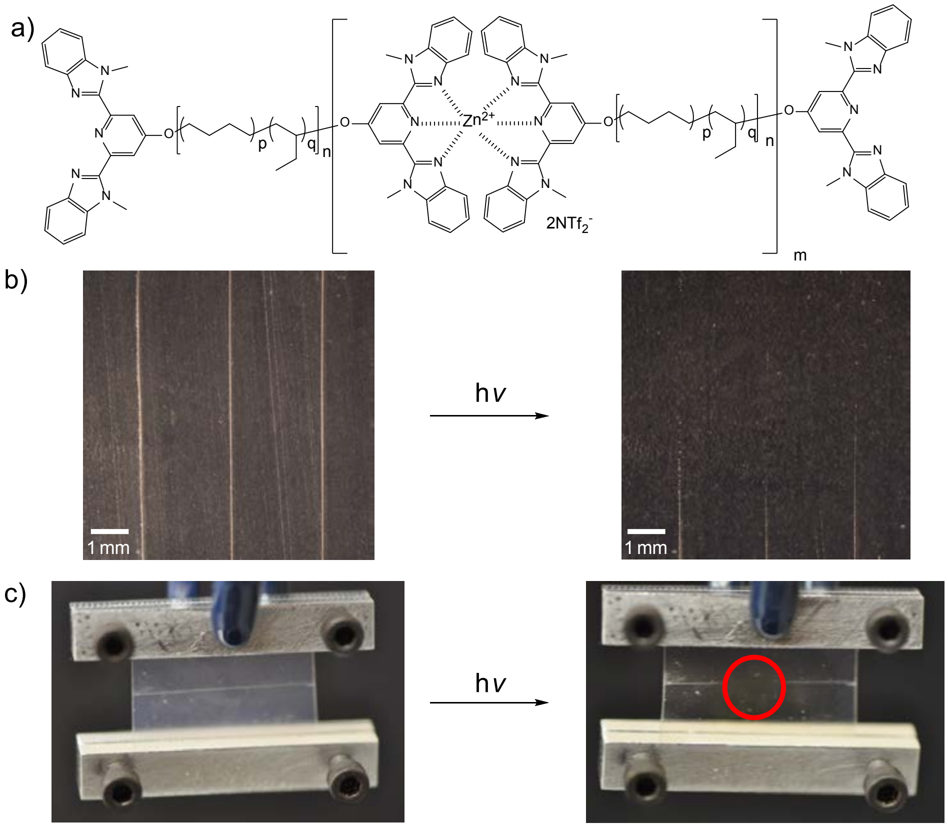

FIGURE 10

Photo-healable metallo supramolecular polymer. (**A**) Chemical structure of the photo-healable polymer. (**B**) Optical healing of the polymer upon exposure to light in the wavelength range from 320-290 nm for 35 s twice at an intensity of 950 mW/cm^2. (**C**) Optical healing of the polymer while under load (~8 kPa); red circle shows the approximate area where the beam was focused.

H. High-resolution Real-time Microscopy of Living Cells

Professor Angela Belcher, Massachusetts Institute of Technology, ISN (UARC)

This research effort focuses on an innovative, real-time microscopy method that could provide a unique approach to investigating the mechanisms of action of antibacterial compounds. The fundamental objective of this research effort is to enable real-time imaging of the dynamic cellular processes of whole, live cells at a nanometer resolution. Using an imaging method such as this, investigators could potentially better understand the kinetics of individual bacterial cell death and mechanisms by which bacteria gain resistance to certain compounds, as well as study compounds that show improved antibacterial efficiency and a low propensity for bacterial resistance, relative to existing therapeutics.

ISN researchers have successfully adapted atomic force microscopy (AFM) to produce high-speed, high-resolution videos of bacteria under attack by small proteins called antimicrobial peptides (AmPs). Although AmPs are a promising new class of antibiotics that have the potential to battle resistance in bacteria, traditional approaches have failed to provide conclusive evidence for the molecular mechanisms involved in the bactericidal action. Using this new imaging method, the investigators captured for the first time, at nanometer resolution, the behavior of single cells seconds after injection of an AmP. The results reveal that the AmPs kill bacteria by

disrupting the cell membrane in a series of phases—an incubation phase (seconds to minutes) followed by a more rapid execution phase (see FIGURE 11). A corrugated texture, as shown in the later time points in FIGURE 11, indicates that the cell membrane is damaged and the cell has died, as was confirmed by other analysis methods (see FIGURE 12).

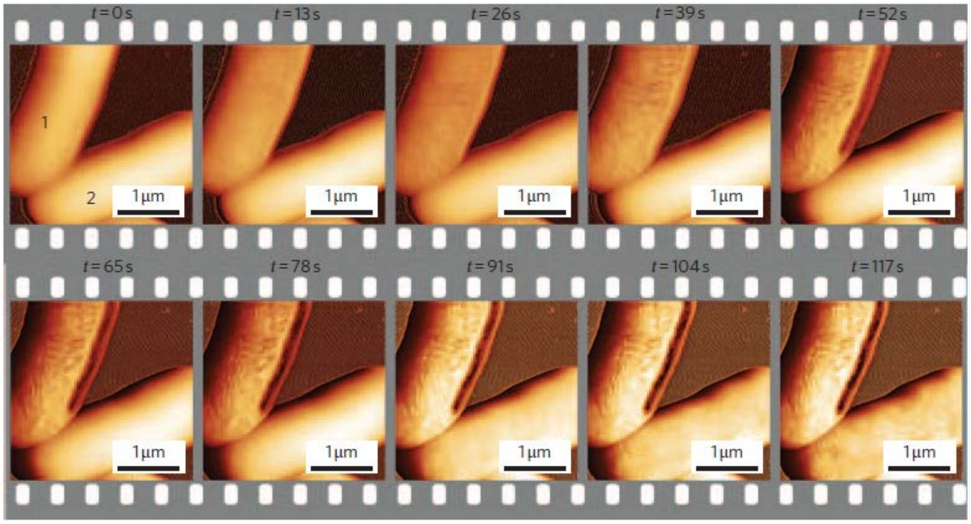

FIGURE 11

Time series of AmP antimicrobial action on *E. coli*. As shown in these selected frames from the video microscopy analysis, the normally-smooth membrane surfaces of the bacteria (t=0s) begin changing to a rough, corrugated texture (t=26s for bacterium 1), with both bacteria in the image displaying significantly-damaged membranes after nearly 2 min of exposure to an AmP (t=117s). A corrugated texture indicates that the cell membrane is damaged and the cell has died. A similar analysis using cells treated with a traditional antibiotic (ampicillin) revealed only minor changes to the cell membranes visible after 112 minutes of exposure.

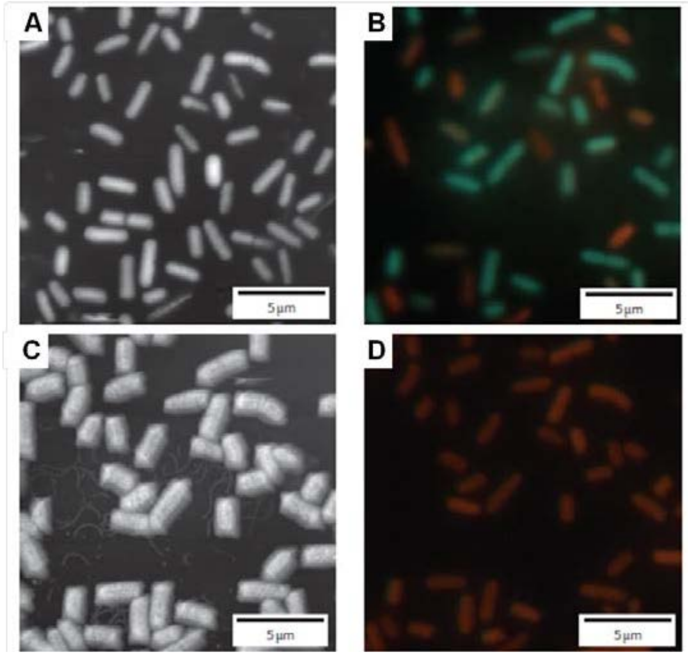

FIGURE 12

Combined AFM and fluorescence microscopy images recorded on the same spot before and after addition of an AmP. (A) Tapping-mode image of bacteria before the addition of AmP shows that the surfaces of most bacteria are smooth. (B) Fluorescence image before the addition of AmP. Live bacteria=green; dead bacteria=red. (C) AFM image 30 min after exposure to an AmP solution at 2x the minimum inhibitory concentration revealed that most bacteria had a corrugated surface. (D) Fluorescence image after the addition of AmP revealed that all bacteria are red, indicating death. AFM images were taken with a resolution of 512 x 256 pixels and a scan rate of 0.5 Hz.

Prior to this work, high-resolution AFM imaging of live cells had been limited to longer acquisition times (several minutes per image), while high-speed AFM imaging had been limited to viewing small areas and flat samples. Additionally, imaging live bacteria in an aqueous environment has proven very challenging with conventional cantilevers. The investigators overcame these scientific barriers by using micro-fabricated small cantilevers, with a mass approximately one thousand times smaller than that of conventional cantilevers, to enable high-speed imaging in tapping mode, while limiting the AFM tip force exerted on the bacteria (see FIGURE 13).

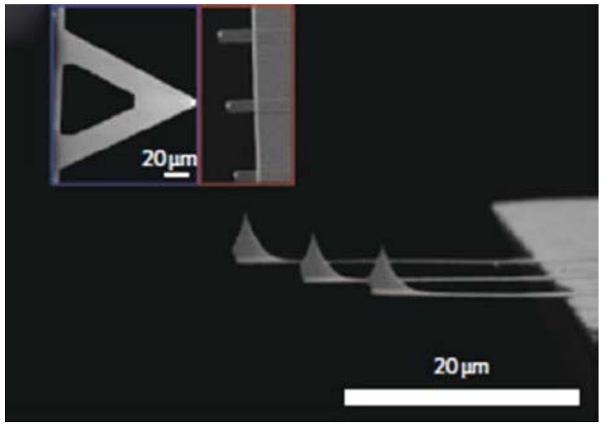

FIGURE 13

Small AFM cantilevers for high-speed AFM. Scanning Electron Microscope (SEM) image of small silicon nitride cantilevers (approximately 10 mm wide, 100–350 nm thick, 20–30 mm long). The inset compares the small levers (right) and a conventional lever (left) used for AFM imaging in fluid at the same magnification.

The key benefit of this instrument is the combination of very soft but rapid imaging and a scan size large enough to monitor multiple cells simultaneously. These measurements demonstrate the enormous potential of high-speed AFM imaging for cellular biology. This technique can be applied to other cell types such as yeast or mammalian cells and even to eukaryotic cell organelles. The advances in AFM technology and its application reported here constitute an enabling technology with which cell biologists may explore cellular processes, in real time, at the nanometer level.

The long-term applications of this research for the warfighter could include the development of a new class of highly-potent antibiotics, improved dressings for wound healing, bacterial-resistant clothing, and improved packaging for food preservation.

I. Studying Novel Electrocatalysis under Alkaline Conditions

Professor Sanjeev Mukerjee, Northeastern University, Single Investigator Award

Professor Mukerjee's study of transition metal homogeneous redox process coupled with heterogeneous electron transfer reactions has enabled the synthesis of novel electrocatalysts for the anodic oxidation of complex fuels (especially directed towards facile breakage of C-C bond). This research is attempting to understand electrocatalysis under alkaline conditions. He is using a variety of electrochemical and spectroscopic techniques to understand adsorption and activation of chemical species on complex metal surfaces. The investigator's research consists of three main tasks: (i) synthesis of electrocatalysts, both supported and unsupported on various carbon blacks using a variety of novel synthetic approaches, (ii) measuring electrocatalytic activity using a specially designed RRDE set up to investigate the kinetic parameters and parallel electron transfer step (at the ring electrode) while avoiding the interference from factors such as carbonate formation (in the case of anodic oxidation of alcohols) using specially designed protocols, and (iii) in situ XAS investigation of electrocatalytic pathways using newly developed technique referred to as '$\Delta\mu$ technique' enabling site specific adsorption of moieties to be determined.

A novel approach of heterogeneous electron transfer reactions coupled to homogeneous redox process was utilized to significantly alter the mechanism of ethanol oxidation at platinum surface sites. A TM(IV) (transition metal) acetate was added into the system of 0.25 M KOH containing 1M ethanol during electrochemical

measurement. Cyclic voltammetry and chronoamperometry tests were done at room temperature. FIGURE 14 shows the onset potential for ethanol oxidation in the presence of TM(IV), predominated beyond 0.3V vs. RHE, indicating a promoting effect of the TM(IV) on ethanol oxidation. Differential electrochemical mass spectrometry was conducted using ^{13}C labeled ethanol to confirm C-C bond cleavage of ethanol with and without co-catalysts. FIGURE 15 shows the fraction of the $^{13}CO_2$ in all CO_2 released from the aliquot volume of the electrolyte solution upon acidification. There is a notable difference in the $^{13}CO_2$ levels and therefore in the extent of the (electro) catalytic cleavage of C-C bond in presence and absence of TM(IV) based co-catalysts indicating that these systems are capable of fully oxidizing ethanol to carbon dioxide at room temperature.

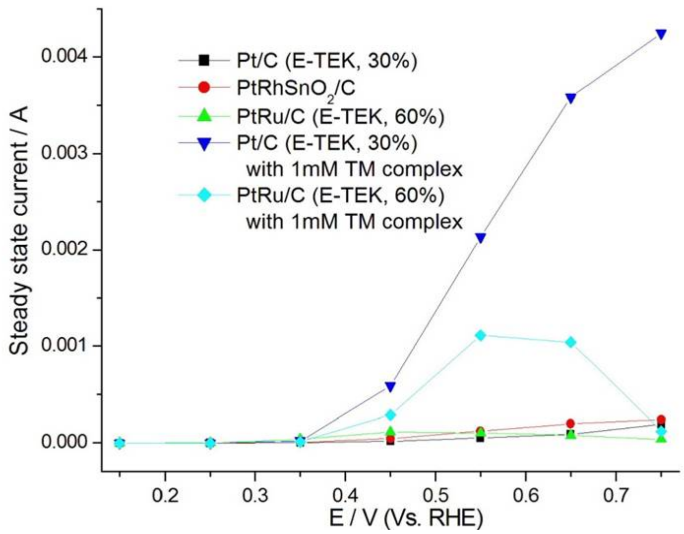

FIGURE 14

Onset potential for ethanol oxidation in the presence of a transition metal complex. Steady state polarization measurements for electrocatalysts on glassy carbon electrode (Pt loading 15µg/cm2) as a function of potential in 0.25 M KOH plus 1 M ethanol is plotted, showing that the presence of the transition metal complex dramatically enhanced ethanol electro oxidation while those catalysts without the transition metal complex show little activity.

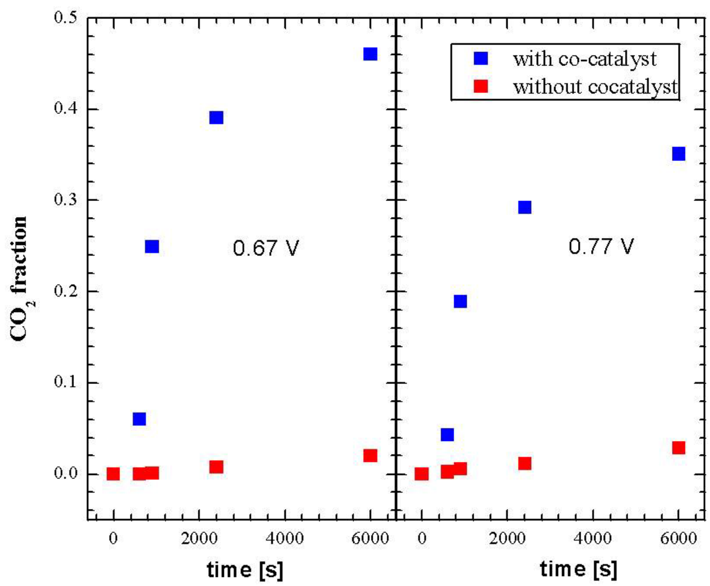

FIGURE 15

$^{13}CO_2$ fraction released from the aliquot volume of the electrolyte solution upon acidification. CO_2 fraction measured during ethanol oxidation on a porous electrode containing Pt/C (0.4 mg/cm^2, 30% Pt on C, ETEK commercial) at room temperature using ^{13}C labeled ethanol (1 M) plus 0.25 M KOH at two different potentials with and without transition metal (IV) co-catalyst demonstrating that these catalyst systems are capable of fully oxidizing ethanol to carbon dioxide at room temperature.

Professor Mukerjee has developed a co-catalyst with 10 fold enhancement of ethanol oxidation with concomitant evidence of enhanced C-C bind cleavage at near room temperature. This is a tremendous improvement in ethanol oxidation rates over current state of the art electrocatalysts. In current fuel cells, generally high temperatures (above 130°C) are necessary to cleave C-C bonds without deactivating catalysis. A catalyst capable of cleaving C-C bonds at a low temperature can enable the development of low-temp fuel cells that are capable of using complex hydrocarbon fuels, producing low-heat and noise-less power sources, relative to traditional combustion-generator engines.

J. Spectroscopic Investigation of Catalyst Surfaces

Professor Andrzej Wieckowski, University of Illinois, Urbana-Champaign, Single Investigator Award

Professor Weikowski is using use sum-frequency-generation IR spectroscopy (SFG-IR) to characterize catalyst surfaces study the oxidation of ethanol under both acidic and alkaline conditions. The SFG-IR method is only sensitive to molecules on a surface, thus it provides a method to selectively probe adsorbed species.

The team has already characterized all forms of adsorbed CO on single-crystal as well as on polycrystalline surfaces and completed the first-ever SFG measurements of acetate and bisulfate anions on metal surfaces in both acidic and alkaline media (see FIGURE 16). These results enabled the study ethanol oxidation reaction and surface adsorbed intermediates of ethanol with BB-SFG in unprecedented detail. The investigator has also studied ethanol reaction pathways with isotopically labeled ethanol using SFG. The data indicate that adsorbed carbon monoxide primarily comes from the alcohol portion of the ethanol molecule.

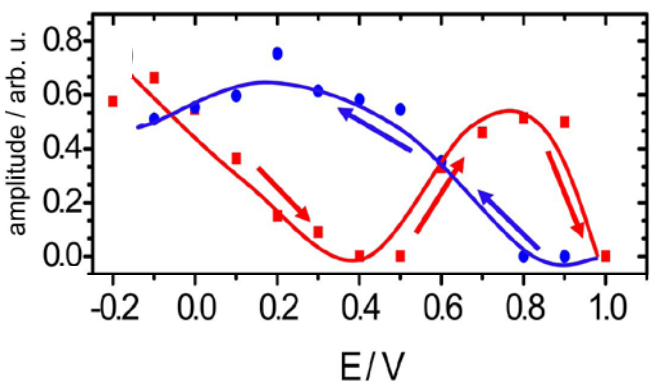

FIGURE 16

CO surface intermediates (from ethanol) on Pt in NaOH. Data show that in the potential window of an ethanol fuel cell (0.3 – 0.5 V on the anodic sweep) the surface is basically CO free and may act as catalytic contamination-free sites. The data indicate the low, overall CO coverage for ethanol oxidation in NaOH (SFG amplitude ≈1/10 compared to $HClO_4$) and that there is low concentration of acetate in the basic media.

Understanding ethanol oxidation on catalyst surfaces is the first step toward enabling the use of complex hydrocarbon fuels in room-temperature fuel cells that could generate power for the dismounted Soldier and reduce Soldier-borne weight.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Enabling Computational Technologies for the Accurate Prediction/Description of Molecular Interactions in Condensed Phases

Investigator: Professor Christopher Cramer, University of Minnesota, Single Investigator Award
Recipient: Various DoD laboratories

The accurate prediction of the free energy of solvation is important because of the considerable importance of solvation as it influences such phenomena as changes in reaction rates and mechanisms, the hydrophobic effect, chromatographic retention behavior, interfacial concentration and transport, protein folding, protein-ligand binding, and pharmaceutical (or toxin) bioavailability.

A new family of continuum solvation models termed SMx (where x is a small integer identifying the particular model) was developed at the University of Minnesota and was shown to have a high degree of accuracy (~ 2 kcal/mole) for predicting the free energies of aqueous solvation for a large training set consisting of organic solutes. The SMx models were coded into many software packages, including several distributed freely, under license by the University of Minnesota. The Cramer group is continuing to incorporate SMx developments into popular quantum chemistry codes such as Gaussian, GAMESS, and Hondo. There are ongoing developmental relationships with the commercial distributors of JAGUAR and Q-CHEM, and solvation models will be made available in these software packages as well. This year, the solvation model SMD was incorporated into Gaussian 09 and further contributions are anticipated to be made to Gaussian as code development proceeds. In addition, this transition has led to the active use of these solvation models by Army scientists at the ARL Weapons and Materials Research Directorate (ARL-WMRD), the U.S. Army Corps of Engineers, and the Air Force Research Laboratory (AFRL).

B. Optimal Dynamic Detection of Explosives

Investigator: Professor Hershel Rabitz, Princeton University, Single Investigator Award
Recipient: ARL-SEDD

This research is focused on the optimal dynamic detection of explosives (ODD-Ex). This approach involves controlled quantum interferences and subsequent detection utilizing electromagnetic resources ranging from the UV to the microwave regime, thereby drawing on the best capabilities of these methods in several modes of operation. The research rests on a theoretical and conceptual foundation based on the control of wave phenomena. The ODD-Ex technique relies on the utilization of optimally shaped laser pulses to simultaneously enhance sensitivity to explosive signatures, while reducing the influence of noise and the signals from background interferents in the field. A molecular dynamics research group at ARL-SEDD has procured a femtosecond laser and the necessary supporting equipment to construct an ODD-Ex test facility. With the technical support of staff from the Rabitz group at Princeton, the latest ODD-Ex methods and technology have been transitioned to ARL-SEDD. This will provide the Army with the ability to utilize and apply ODD-EX for the testing and design of future field applications.

C. Elucidating Reactivity and Potential Antimicrobial Action of Conjugated Polyelectrolytes

Investigator: Professor David Whitten, University of New Mexico, DTRA Award
Recipient: NSRDEC

Professor Dave Whitten is currently studying conjugated polyelectrolytes as potential sensitizers of reactive oxygen intermediates in both light-activated and dark processes. A variety of polycationic- and polyanionic-conjugated molecules and polymers have been synthesized (see FIGURE 17). These molecules were found to exhibit significant anti-bacterial activity when tested against vegetative cells in both light and dark reaction

conditions. To exploit the unique properties of these molecules, the group has created tiny microscopic spheres or hollow conjugated polyelectrolyte capsules that trap and kill harmful bacteria, similar to "roach motels", and have successfully demonstrated capture and kill of *B. atrophaeus* spores. These results have transitioned to NSRDEC, and continuing joint research between the PI and NSRDEC is exploring these conjugated polyelectrolyte systems as sporicidal agents on rayon and cotton fabric supports.

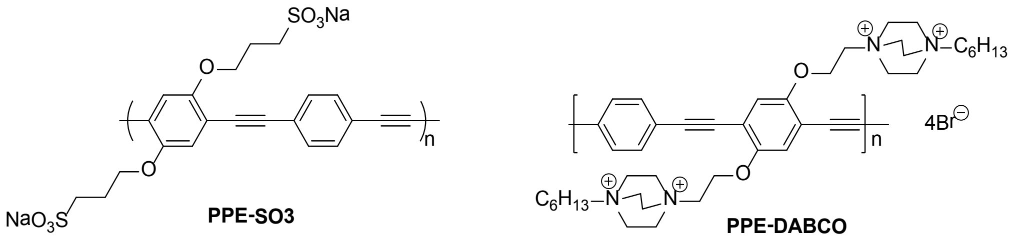

FIGURE 17

Conjugated polyelectrolytes. These polycation and polyanion conjugates were found to have antimicrobial and sporicidal activity, and will be further tested at NSRDEC.

D. Catalytic Decontamination: New Systems and Fundamental Studies

Investigator: Professor Craig Hill, Emory University, Single Investigator Award
Recipient: ECBC

The objective of this research is to explore the physical and chemical properties of new metal oxide and metal catalysts with a focus on their ability to transform hazardous chemicals into relatively benign substances. The investigator has developed highly active catalysts for the oxidation of 2-CEES, a chemical weapon simulant. The catalysts are transition metal oxide-anion clusters called polyoxometalates (POMs; see FIGURE 18), substituted at surface sites with Cu or related metals that bear terminal NO_x ligands such as $[H(ONO_2)_2]^-$. These catalysts do not require addition of a stoichiometric oxidant and are stable under typical environmental conditions. The Hill group has recently started to incorporate these POM-based catalysts into metal-organic frameworks (MOFs). The hybrid materials take advantage of the sorption properties of the MOF and the catalytic properties of the POM. These materials have transitioned to the filtration group at ECBC for advanced adsorption testing in air filtration applications.

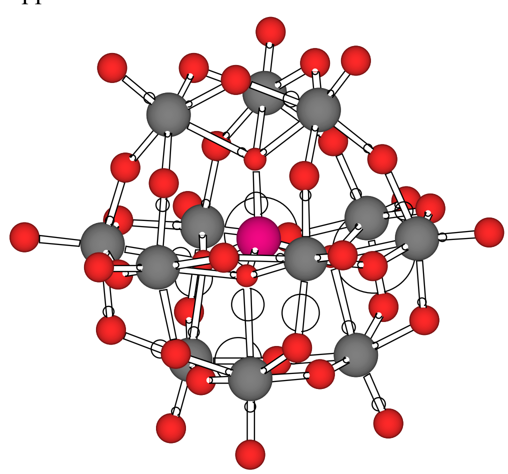

FIGURE 18

Polyoxometalate structure. This transition metal oxide-anion cluster has the capability of catalyzing detoxification reactions of hazardous chemicals. These structures have transitioned to ECBC for testing in potential air-filtration applications.

E. Sorbent Materials and Mechanisms of Removal
Investigator: Professor T. Bandosz, City College of New York, Single Investigator Award
Recipient: ECBC

The objective of this research is to explore novel carbon-based materials and probe the chemical and physical properties that control adsorption and transport. The Bandosz group has developed carbon-based composite materials based on activated carbons, graphite oxide, MOFs, and transition metal catalysts for reactive adsorption of toxic industrial chemicals, including ammonia. The researchers found that graphite oxide and MOF-composite materials have increased porosity and enhanced adsorption capabilities over the single-component materials and physical mixtures (see FIGURE 19). These materials have transitioned to the filtration group at ECBC for advanced testing of their adsorption capabilities of ammonia and other toxic industrial chemicals.

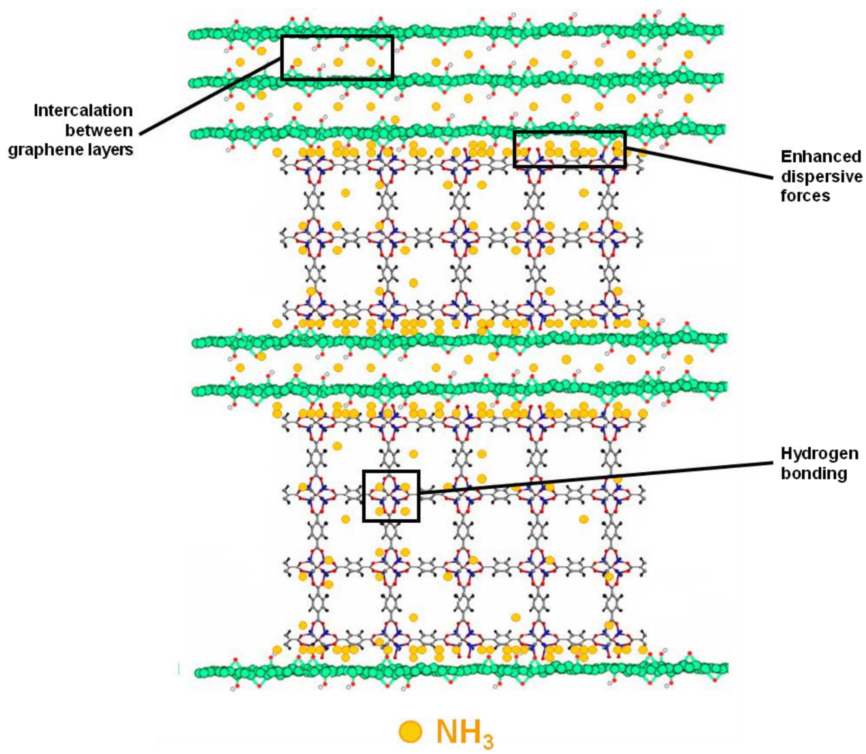

FIGURE 19

Graphite-oxide MOF composite. This composite material was found to have enhanced adsorption capabilities relative to the single-component materials and physical mixtures. Proposed sites for ammonia adsorption are indicated in the schematic.

F. Bio-templated Synthesis of Janus Nanorods
Investigator: Professor Qian Wang, University of South Carolina, Single Investigator Award
Recipient: NSRDEC and the Naval research Laboratory

The focus of the research effort led by Professor Wang is to design and synthesize novel hierarchical nanostructures with distinctive surface properties at each end. Two rod-like viral particles (rVP) are being explored in this study: tobacco mosaic virus (TMV) and bacteriophage M13. The intrinsic self-assembly properties of TMV and M13 and bioconjugation techniques developed in the investigator's laboratory are being used to prepare the particles. During the past year, the group has successfully generated several TMV mutants, has investigated the conjugation reactivity of the M13 phage, and has prepared TMV-rVPs with well-defined lengths. The researchers are carrying out joint research with NSRDEC to prepare virus-based materials for sensing and tissue regeneration. A new approach to surface modification of the M13 bacteriophage, developed in the investigator's laboratory, was transitioned to NSRDEC for testing in neurotoxin-detection applications. In addition, the Naval research Laboratory (NRL) is interested in these results and the investigator is synthesizing

TMV-templated conductive nanowires for analysis. A student from the investigator's laboratory was also recruited by NRL to be a post doctoral researcher.

G. Multiscale Simulations of Barrier and Aging Properties of Polymer Nanocomposites
Investigator: Professor Venkat Ganesan, University of Texas – Austin, Single Investigator Award
Recipient: ARL-WMRD

The focus of the research effort led by Professor Ganesan is to develop a multiscale simulation approach that can be used to obtain a fundamental understanding of the origins and the design parameters underlying the barrier properties of polymer nanoparticle composite membranes and their time evolution (aging properties). A computer simulation module was developed and transitioned to ARL-WMRD that is capable of predicting the structure and rheology of multicomponent polymers. A graduate student spent two months at ARL-WMRD to adapt the coarse-graining methodology to problems of Army interest. In addition the principal investigator visited ARL-WMRD twice and presented seminars to discuss opportunities for interactions.

H. Solider Power Manager
Investigator: Protonex Corporation, SBIR contract
Recipient: 2nd Brigade, 2nd Infantry Division

Through an SBIR contract, research led by Protonex Corporation focused on developing technologies that would allow fuel cells and other alternative power sources to be used with a variety of power using devices with varying voltage and current requirements.

This research led to the development of the Soldier Power Manager (SPM), which is a power-converting device that actively "takes the power you have, and delivers the power you need." It is used to power virtually any piece of portable military/commercial gear from any available battery and to charge any military/commercial rechargeable battery. The warfighter does not need to know anything about the power requirements of the equipment; the Soldier simply uses a smart cable to connect gear to the SPM and the correct voltages and currents are automatically generated. The SPM reduces the number and quantity of batteries being used and also take advantage of non-traditional energy sources. For example, they can be used with fuel/solar cells to lengthen intel missions, where the mission duration is limited by power.

Six SPMs were transitioned to Operation Iraqi Freedom, providing the warfighter the capability to power portable military/commercial gear from any available battery or to charge any rechargeable battery. In this case the SPMs were used in conjunction with Ultracell fuel cells (from a CERDEC program) to allow the fuel cells to be used with a variety of U.S. Army equipment.

I. Direct Complex Hydrocarbon Oxidation Catalyst
Investigator: Professor Sanjeev Mukerjee, Northeastern University, Single Investigator Award
Recipient: ARL-SEDD

Professor Mukerjee's research is exploring electrocatalysis under alkaline conditions. He is using a variety of electrochemical and spectroscopic techniques to understand adsorption and activation of chemical species on complex metal surfaces. This ARO sponsored research at Northeastern University developed a new alkaline electro oxidation catalyst capable of cleaving carbon-carbon bonds at near ambient temperatures, which could allow the development of low-weight fuel cells for the warfighter. The researchers have characterized the catalyst's structure, identified the mechanism of action, and demonstrated the complete oxidation of ethanol fuel. These results are a critical step in enabling the use of complex fuels in ambient temperature fuel cells, which could ultimately be used to reduce Solider-borne weight. These efforts transitioned to ARL-SEDD through on-site research carried out by a member of the research team who spent six weeks at ARL-SEDD characterizing the catalysts, their ability to fully oxidize complex hydrocarbon, and the tolerance of fuels to sulfur.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Radical Reactions in the Decomposition of Energetic Compounds
Professor Laurie Butler, University of Chicago

The study of chemical phenomena occurring during explosions has been hindered by the difficulty of isolating and/or detecting reactive radical intermediates and products. The measurement of product velocity and angular distributions in a state-of-the-art crossed laser-molecular beam apparatus overcomes this obstacle and incorporates specific capabilities crucial to elucidating the dynamics of both the photolytic generation process and the branching between competing product channels of the radical intermediates (see FIGURE 20).

In FY11, the crossed laser-molecular beam apparatus will be used to study the H_2CNO_2 radical in a molecular scattering apparatus in order to determine the energetic onset of the NO and NO_2 products. The CH_2NO_2 radical serves as a model system for primary radicals generated from the decomposition of 3-nitro-1,2,4-triazol-5-one (NTO) and 1,3,3-trinitroazetidine (TNAZ). The energetic onset of each product channel offers a determination of the nitro-nitrite isomerization barrier and the C-NO_2 bond fission barrier in the radical. This information will be important for understanding how energetic compounds containing nitro groups decompose during the detonation process. The results will also offer a definitive benchmark for electronic structure calculations of the transition states, relevant to the dissociation of open-shell species with nitro groups.

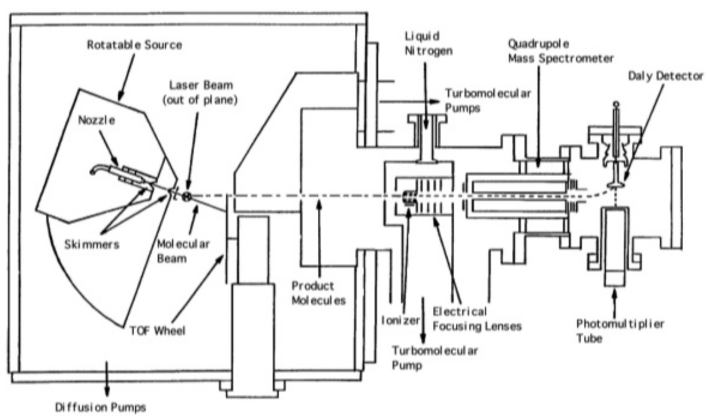

FIGURE 20

Crossed laser-molecular beam scattering apparatus. The measurement of product velocity and angular distributions in this apparatus overcomes the obstacle of isolating and/or detecting reactive radical intermediates and products.

B. New Metal-Organic Polymers through Sub-Component Self-Assembly
Professor J. Nitschke, University of Cambridge

Professor Nitschke is exploring novel metal-mediated reactions to design and synthesize modular, conjugated metal-containing self-assembled polymers. This approach, referred to as sub-component self-assembly, involves covalent (carbon-heteroatom) and dative (heteroatom-metal) reversible bond formation from basic building blocks and metal-ion templates. The building blocks (typically Cu-N, where N is imine or pyridine) are designed to provide unique functionality and ultimately, new molecular architectures. Preliminary results indicate that the materials have an increased stability to hydrolysis and nucleophilic cleavage.

A variety of new materials will be synthesized via this sub-component self-assembly approach, including double-helical polymers, metal organic polymers, and triple-stranded ladder polymers, and their chemical and physical

properties will be explored (see FIGURE 21). Conductance and redox potentials for these materials will be determined in the next year. These unique materials will possess desirable properties including dynamic reconfiguration, high strength, or conducting behavior for relevant Army and DoD applications in self-healing materials, armor/protective clothing, and sensing.

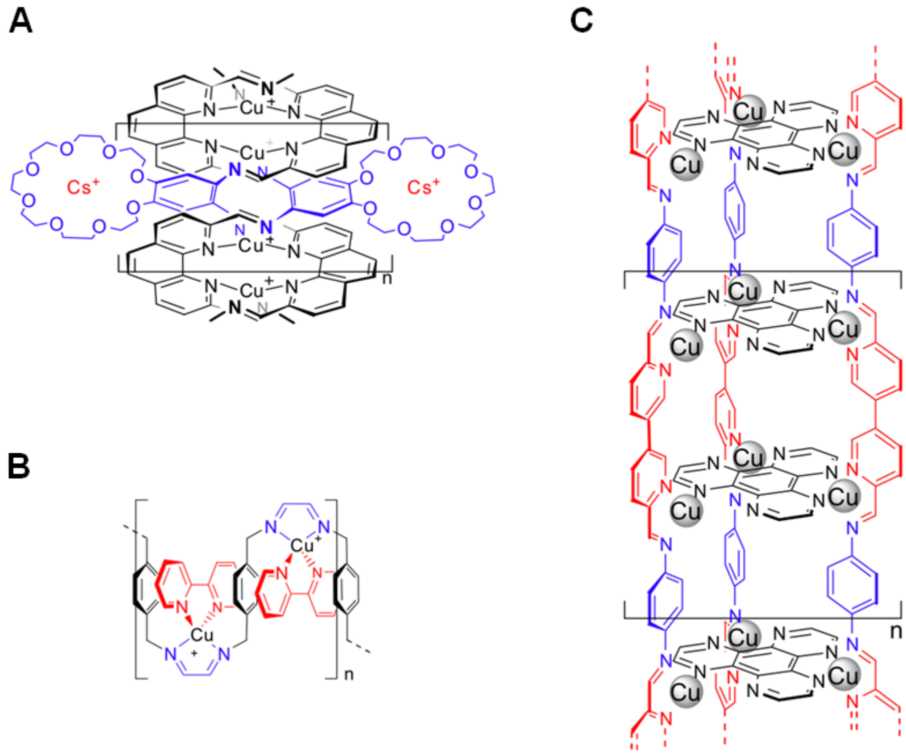

FIGURE 21

Examples of polymer structures. Using the sub-component self-assembly approach, a variety of new materials will be synthesized, including (**A**) double-helical polymers, (**B**) metal organic polymers, and (**C**) triple-stranded ladder polymers.

C. Precision Morphology in Sulfonic, Phosphonic, Boronic, and Carboxylic Acid Polyolefins

Professor Kenneth Wagener, University of Florida, Gainesville

The biggest scientific challenge of this project has been to generate precisely placed sulfonic acid groups along the polymer backbone. Researchers have successfully accomplished this for carboxylic acids and for phosphonic acids, but not yet for the sulfonic acid group. Protecting the sulfonic acid functional group is essential for a successful polymerization. Esters have been examined thoroughly as protecting groups. Although it might seem to be trivial to remove these esters, only a partial deprotection occurs and the polymer then precipitates, thus terminating the reaction. Recently, the investigator has initiated a series of thermal deprotection studies on model compounds (see FIGURE 22). These studies demonstrate the formation of sulfonic acids with isobutylene released as a gas. In the coming year it is expected that this approach will be applied to polymer chemistry to generate the first ever precision polyolefin with precisely-placed sulfonic acid groups located at either exact or variable locations along the backbone.

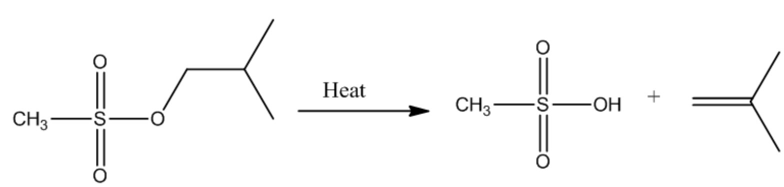

FIGURE 22

Sulfonic acid protection/deprotection. This model system is being used to study sulfonic acid protection/deprotection reactions demonstrates the formation of sulfonic acid with isobutylene released as a gas.

D. Understanding Ion Transport under Alkaline Conditions in Polymeric Materials

Professor Andrew Herring, Colorado School of Mines

Ion transport in complex heterogeneous organic media is ubiquitous to many important energy-conversion devices, particularly fuel cells that have the potential to revolutionize energy conversion. However, ion transport is still poorly understood in terms of its relationship to water content, morphology and chemistry. While a large amount of research has been performed for proton exchange membranes, little work has been performed with anion exchange membranes. These systems are particularly interesting in that the charge carrier may be hydroxide, or carbonate. It is not sufficient, however, to simply understand anion transport in these systems, as robust thin films that have high ionic conductivity must also be fabricated for practical applications.

Professor Herring is leading a team to develop new polymer architectures, and then use a predictive multi-scale computational approach to probe both anion transport and its coupling to polymer morphology in these architectures, followed by a characterization of anion transport. The synthetic work will prepare stable cations, vary modes of attachment to polymer backbones, and generate controlled morphologies. Synthesis and characterization will be tied closely to theory through model validation by the study of aqueous solutions of representative cations and by the study of well-defined polymer architectures. At the molecular-scale a generalization of a novel reactive molecular dynamics methodology will be developed, while more statistical characterizations of ion transport will be implemented on the scale of the membrane thickness.

In the coming year, the resulting novel films will be studied in terms of the anion species present, and their transport and equilibria properties. Water content will be measured by dynamic vapor sorption. Bulk transport will be studied under condition of accurately controlled temperature and relative humidity. This will be complemented by the measurements of self diffusion coefficients and molecular-scale activation energies. Extensive mechanical and rheological testing will be used to develop robust thin films. Morphology will be related to film mechanical properties through state of the art measurements and film degradation will be studied in depth. This research may lead to many Army applications, including the development of alkaline fuel cells to reduce solider weight as well as new materials with selective transport that could be used in advanced sensors or chemical protective equipment.

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CHAPTER 4: COMPUTING SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Computing Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to provide increased performance and capability for processing signals and data, extract critical information and actionable intelligence to enhance the warfighters' situation awareness, improve decision making, and improve weapon systems performance. The Division supports basic research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and techniques governing intelligent and trusted computing systems. More specifically, the goal of the Division is to promote basic research to establish new computing architectures and models for intelligent computing, to create novel data fusion and extraction techniques for efficient information processing, and to build resilient computing systems for mission assurance. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of computing sciences research.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of computing science, the research efforts managed in the Computing Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. This program identifies and addresses the Army's critical basic research problems in the computing sciences where progress has been inhibited by a lack of novel concepts or fundamental knowledge. The transformation of the Army to the Future Force will require investment in science and technology, especially computing and information science. Computing science is pervasive in nearly all Army systems, particularly Command, Control, Communications, Computing, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems. The number of information sources on the battlefield will grow rapidly; computing and information science research must provide the technology to process this in real-time and ensure that Soldiers and commanders do not experience information overload that could adversely affect their ability to make decisions. Also, in spite the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. For this reason, computing science is a key technology underpinning the Future Force. The research topics described here are needed to provide the Future Force the information processing, computing, security, and reliability needed to achieve the vision of future Army operations. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals.

3. Coordination with Other Divisions and Agencies. The Division research investment strategy is coordinated with partner disciplines and computer scientists at ARO, other directorates within ARL, other Army agencies, and related programs in other DoD and Federal agencies. The Division research portfolio is supported by Army basic research Core funding with substantial additional resources from the Director Defense Defense Research and Engineering (DDR&E), including the Multidisciplinary University Research Initiative Program (MURI), and from other agencies, such as the Defense Advanced Research Projects Agency (DARPA), the Department of Homeland Security (DHS), and the National Security Agency (NSA).

To effectively meet Division objectives and to maximize the impact of potential discoveries for the Army and the nation, the Computing Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers and with researchers in other DoD agencies. In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate effective human computer communication mechanism. A successful research outcome may lead to a revolutionarily new way for human communications. The Division also coordinates efforts with the Network Sciences Division to explore new techniques for robust and resilient mobile ad hoc networks, to establish adversarial models for effective cyber defense, and to investigate fundamental principles for trusted social computing. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas. Each of the Program Areas within the Division balances opportunity-driven research with high risk, high-payoff scientific exploration and needs-driven efforts that look for solutions to the near-term needs of the warfighter.

B. Program Areas

To meet the long-term program goals described in the previous section, the Computing Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these three Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, and (iii) Information and Software Assurance. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Information Processing and Fusion. The goal of this Program Area is to understand the fundamental principles and to establish innovative theories for data processing, information extraction, and information integration toward real-time situational awareness and advanced targeting. There are five Thrusts for this Program Area: (i) mathematical image processing, (ii) image understanding, (iii) data and information fusion, (iv) target acquisition and tracking, and (v) brain-computer interfaces. With the pervasive availability of unmanned systems in future military operations, advanced sensing will be of critical importance to the future force. This program emphasizes mathematical methodologies underlying automated sensing and scene understanding. Research efforts support the development of novel algorithms for robust video-based tracking under challenging urban environments. Also supported is research on area monitoring using a network of cameras and other sensing modalities. Potential applications include detection of improvised explosive devices and persistent surveillance. There is also a new research initiative on brain signal understanding for brain-computer interfaces using both minimally invasive and non-invasive imaging modalities.

The increased capability of electronic systems and the proliferation of sensors are generating rapidly increasing quantities of data and information to the point that system operators and commanders are overwhelmed with data and saturated with information. An area of increasing importance is data and information integration or fusion, especially fusion of data from disparate sensors and contextual information. Research activities address several basic issues of data fusion, including information content characterization of sensor data, performance modeling, and the value of information.

2. Computational Architectures and Visualization. The two main Thrusts of this program are Computational Architectures (CA) and Visualization (V). The goal of the CA Thrust is to discover new effective architectures, computational methods, and software tools for future computing systems with special emphasis on the effect that the technological shift to heterogeneous, multi-core processors will have on newly-developed systems. The goal of the V Thrust is to make very large simulations and the visualization of massive data sets more computationally efficient and more interactive for the user. An overarching theme for both Thrusts is the efficient managing and processing of massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, and visualize such massive amounts of information. The CA Thrust attempts to address this issue by investigating innovative architectural designs of both hardware and software components and their interfaces.

The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

The long-term payoffs of the CA Thrust for the Army include new computer modeling and design concepts (or paradigms) as well as software libraries that take advantage of these new multi-core processors and that are scalable (usable on large-scale complex problems and able to handle massive amounts of data) and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. A payoff associated with the V Thrust is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

3. Information and Software Assurance. The goal of this Program Area is to understand the fundamental principles of robust and resilient systems that can enable the corresponding functions to be sustained under adversarial conditions. The studies guided by this program will enable and lead to the design and establishment of trustworthy computing and communication, regardless of threat conditions. The ARO program on Information Assurance currently has two major Thrust areas: (i) Highly Assured Tactical Information and (ii) Resilient and Robust Information Infrastructure. The goal of the Highly Assured Tactical Information Thrust is to gain new scientific understandings for trustworthy tactical communications and for establishing fundamental principles and models for robust and resilient tactical information processing. The Resilient and Robust Information Infrastructure Thrust promotes research efforts on cyber situation awareness theory and framework, which combines intrusion prevention, detection, response, and recovery together and establishes fundamental scientific principles for building mission-sustaining information systems (*e.g.*, software/hardware, computing/communication systems).

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-off among performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques to obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and the impact on cyber missions, and model the behavior of adversaries to predict the threat of future attacks on the success of a mission. Information assurance for the individual Soldier and for the systems that the Army must employ in the next few years is of paramount importance to the defense of this nation. The Objective Force must have unprecedented situational awareness (including enemy and friendly awareness) at all times. It follows then, from the Army perspective, that Information Assurance must address the delivery of authentic, accurate, secure, reliable, timely information, regardless of threat conditions, over heterogeneous networks consisting of both tactical (mobile, wireless) and fixed (wired) communication infrastructures. As the Army places more reliance on winning the information war and providing the Soldier with highly automated and sophisticated tools, there must be an increased and improved awareness of the vulnerabilities that these systems possess. Ubiquitous, mobile, wireless, scalable, high-speed, and highly assured information processing systems will be placed in areas of usage never imagined in the past. Attacks on these systems will occur from hostile forces in both time of war and time of peace.

C. Research Investment

The total funds managed by the ARO Computing Sciences Division for FY10 were $22.2 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $3.2 million. The Department of Defense Multi-disciplinary University Research Initiative (MURI) and Defense University Research Instrumentation Program (DURIP) provided $7.8 million to programs managed by the Computing Sciences Division. The Small Business Innovation Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $3.3 million for awards in FY10. In addition, congressional earmarks provided $7.7 million. Finally, $0.2 million was provided from other sources for use in specific programs, including the Presidential Early Career Award for Scientists and Engineers (PECASE) program and the Historically Black Colleges and Minority Institutions (HBCU/MI) program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. ARO Special Workshop on Computing with Social Trust (College Park, MD; July 29-30 2010). One of the important social factors in many decision-making applications is *social trust*. In many computing systems, information is produced and processed by many people, and knowing how much a user trusts an information creator can be very useful for aggregating, filtering, and ordering of information. If social trust is used to support decision making, it is important to have an accurate estimate of trust and confidence when it is not directly available. The trust estimates must be computed efficiently, since most realistic decision-making applications involve massive amounts of data and large networks of people. This workshop brought together experts in academia, industry, and government laboratories to discuss the critical problem of computing with social trust, covering semantics, algorithms, relationship analysis, and theoretical and logical foundations of trust. New research opportunities and challenges were identified at the workshop.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Computing Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Sensor Network Structure for Dependable Fusion. This MURI began in FY07 and was awarded to a team lead by Professor Shahi Phoha at the Pennsylvania State University. The goal of this research is to develop theoretical foundations and validation to address: (i) proliferation of multi-source sensor data due to DoD's tactical shift to network-centric warfare, (ii) urban area monitoring demands for fighting the asymmetric warfare, and (iii) collaboration needs of future military devices or systems.

The emphasis of these studies is on network science, which enables construction of sensor networks to support dependable information fusion. The research is based on fundamental concepts of space-time neighborhoods in the vicinity of events, symbolization, nonlinear filtering, and computational geometry to formulate rigorous mathematical methods and algorithms to capture the causal dynamics of distributed information fusion processes

in urban sensor networks. These studies could potentially lead to robust and resilient sensor networks for monitoring a given urban area in support of defense missions.

2. Brain-to-muscle Communication. Two MURIs in this topic area began in FY08, with one research team led by Professor Gerwin Schalk at Albany Medical College, and the other team led by Professor Michael D'Zmura at the University of California, Irvine. The objective of these MURIs is to understand the mechanisms of brain nerve-to-muscle signaling so that brain signals can be exploited to provide an accurate, real-time assessment of the user's intentional focus, eye movements, and imagined speech. The effort focuses on three research areas: (i) the methods and algorithms for decoding brain signal recordings of brain cortical activity during covert speech, (ii) communication of covertly-spoken thought using an augmented-reality audio system with a spatialized speech channel, and (iii) exploitation of brain signals for interface design and the development of algorithms using only non-invasive recordings. These studies could potentially lead to a silent, brain-based communication and orientation system to provide a communication channel between humans and computers and improved human-computer interfaces.

3. Principles for Robust and Resilient Tactical Mobile Ad-hoc Networking Systems (MANETs). Two MURIs in this topic area began in FY08, with one research team led by Professor Vigil Gligor at the University of Maryland and the other led by Professor Prasant Mohapatra at the University of California, Davis. The goal of these MURIs is to use insights from multiple disciplines, such as network science, engineering, mathematical science, and systems theory to develop the analytical models, tools, and mathematical representations for assessing, prescribing, analyzing, and predicting the behavior of robust and resilient mobile ad hoc networks under a total threat spectrum, and to provide security, robustness and resilience for tactical MANETs.

These efforts focus on addressing one of the main research challenges of the Computing Sciences Division, Information and Software Assurance Program, Highly Assured Tactical Information Thrust. The research teams will investigate: (i) mathematical representations and tools for modeling and analysis of resilient and robust MANETs, (ii) theories that explain the MANET layered architecture and cross layer interaction (both intentional and unintentional), (iii) theories that elucidate the relationships and understanding of the trade-offs between fragility and robustness, (iv) interaction of networks, particularly, MANETs, low energy wireless sensor networks, and wired communications networks, and (v) design of MANET survivability algorithms and architecture, resilient management mechanisms, threat spectrum analysis for information applications on MANETs, fault tolerant and attack resilient communication protocols, survivability requirements engineering, and security and trustworthiness in MANETs.

The team led by Professor Gilgor is using a research approach based on the fundamental principles of active protocol monitoring for performance, stability and adversary handling, of employing communication channel diversity for robust end-to-end operation in the face of failures and deliberate attacks, and of exploiting cross-layer interaction for predicting the effects of performance changes caused by layer-specific failures and attacks on end-to-end MANET operation. Design and analysis techniques found in network theory, statistics, game theory, cryptography, economics and sociology, and system theory are used to develop, design and analyze models, tools, and mathematical representations for predicting performance and prescribing resilient, secure MANETs.

The team led by Professor Mohaptra is developing a cross layer architecture that provides comprehensive security and resilience. Depending on the services desired the new architecture will be able to adaptively provide the right trade-offs between performance, security and fault-resilience. The team currently undertakes three parallel but inter-coupled tasks geared towards (i) performing measurements via real deployments and enhancing understanding of layer dependencies and vulnerabilities in mobile ad hoc networks, (ii) building analytical models to characterize the behavioral nuances of these networks, and (iii) designing new cross layer protocols that protect against vulnerabilities and provide the desired robustness.

4. Cyber Situation Awareness. Two MURIs in this topic area began in FY09, with one research team led by Professor Richard Kemmerer at the University of California, Santa Barbara, and the other team led by Professor Peng Liu at the Pennsylvania State University. The goal of these projects is to explore cyber situation awareness theories and frameworks that may support effective defense against cyber attacks, and to develop new algorithms and systems that can assist human analysts' cognitive situation awareness processes and decision making.

Complete situation awareness leads to effective defense and response to cyber attacks, especially those launched by adversaries with state sponsorship. The ability to extract critical information and build intelligence leads to a better capability in attack prevention, detection and response and in sustaining critical functions and services. The team will focus their research in the following key areas: (i) situation (knowledge and semantics) representation and modeling that support multi-level abstraction and transformation of data to intelligence, (ii) information fusion that can effectively combine raw and abstracted intelligence of different confidence levels to support optimal response, (iii) uncertainty management and risk mitigation through probabilistic hypotheses/reasoning and sensitivity control, which uses multi-level statistical analysis to manage incomplete and imperfect situation information, (iv) leverage cognitive science understandings to automate human analysts' cognitive situation-awareness processes (to recognize and learn about evolving situations, to create automated hypothesis generation, and to reason in both pre-attack planning and post-attack response), (v) develop a new framework unifying perception, comprehension, and projection functions and integrating situation recognition, impact assessment, trend analysis, causality analysis, and situation response together, (vi) establish advanced mathematic models for quantitative analysis and assessment of system assurance, and (vii) rapid repair, recovery and regeneration of critical services and functions as part of automatics response to attacks.

In this research, novel situation awareness theories and techniques will be investigated to obtain an accurate view of the available cyber-assets and to automatically determine the assets required to carry out each mission task. A proposed situation awareness framework that ties together cyber assets, cyber configuration, attack impact, threat analysis and situation visualization under cyber mission is illustrated in FIGURE 1.

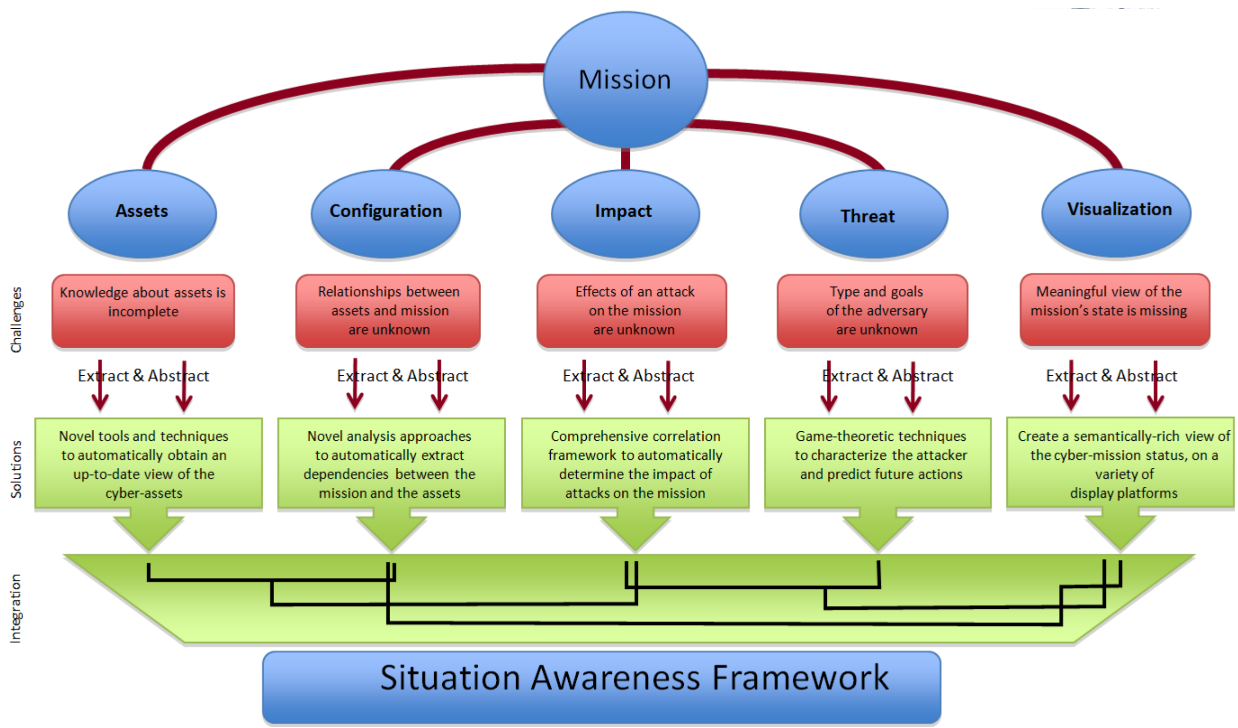

FIGURE 1

Cyber situation framework for attack analysis, prediction, and visualization. This framework incorporates cyber assets, cyber configuration, attack impact, threat analysis, and situation visualization.

5. Principles of Object and Activity Recognition Using Multi-Modal, Multi-Platform Data. This MURI began in FY09 and was awarded to a team lead by Professor Richard Baraniuk at Rice University to gain a fundamental understanding of opportunistic sensing and to create a principled theory of opportunistic sensing that provides predictable, optimal performance for a range of different sensing problems through the effective utilization of the available network of resources.

There are four focus areas in this research focusing on developing a theory of sensing that can provide: (i) scalable sensor data representations based on sparsity and low dimensional manifolds that support

dimensionality reduction through compressive sensing, (ii) scalable data processing for fusing image data from multiple sensors of potentially different modalities for activity detection, classification, and learning, (iii) opportunistic optimization, feedback, and navigation schemes for multiple mobile sensor platforms that adaptively acquire data from new perspectives to continuously improve sensing performance, and (iv) experimental validation on real-world inputs, such as multi-camera video, infrared, acoustic, and human language.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Real-Time Algorithms and Systems for Fused True Color Night Vision Imagery. A Phase II Enhancement SBIR contract was awarded to Opto-Knowledge Systems to develop algorithms and prototype hardware systems for fusing multi-band night vision imagery into a true color display that combines thermal infrared imaging with color low light level imaging. The end result will be camera systems that use intelligent algorithms in real-time to reproduce day or night scenes in natural recognizable colors. These camera systems will generate enhanced imagery for surveillance and reconnaissance, leading to improved scene understanding and reaction time.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Analysis of Target Surface Characterization. A Phase I STTR contract was awarded to Spectral Sciences, Inc., in partnership with Professor Alexei Maradud at the University of California, Irvine, to develop an extended LADAR capability for characterizing and classifying surface material and texture by exploiting multispectral polarimetric LADAR signatures utilizing the Bidirectional Reflectance Distribution Function (BRDF). This innovation will unify waveband spectra, polarization, tomographic reconstruction, and material science with LADAR-based remote target classification. The key features of the capabilities to be developed in this project include BRDF modeling, a database of target and ground materials, range profile simulation, and material inversion algorithms.

2. LADAR Light Reflection Analysis for Target Surface Characterization. This Phase I STTR contract was awarded to System Dynamics, Inc., in partnership with Professor Joseph O'Sullivan at Washington University, to develop and test spectropolarimetric surface characterization algorithms for remote sensing based on Laser Detection and Ranging (LADAR) data. This STTR will utilize a systematic approach that first defines the operational scenarios for which the algorithms are to work. These scenarios are then used to define requirements for LADAR hardware and algorithms, which serves to focus the algorithm development effort. A library of surface material Mueller matrix measurements will be used as the basis for a fundamental surface characterization investigation that will establish the ultimate potential to discriminate between different materials and classes of materials. A preliminary design of improved instrumentation for measuring full Mueller matrix Bidirectional Reflectance Distribution Functions will be made in order to address weaknesses in previous measurement data. Finally, a suite of algorithms will be developed to address the high priority scenarios identified at the beginning of the effort, and these algorithms will be tested on synthetic LADAR images created to represent these scenarios.

3. Multi-input Multi-output Synthetic Aperture Radar with Collocated Antennas. Two Phase I STTR contracts were awarded to Trident Systems Inc. and SA Photonics, Inc. to develop and demonstrate synergistic multi-input, multi-output (MIMO) synthetic aperture radar (SAR) ground moving target indicator (GMTI) capabilities. The goal of these projects is to integrate these sensing technologies so that the tasks of the SAR imaging of stationary targets and background along with SAR-based GMTI, can be performed simultaneously. This major focus of the projects is on a MIMO radar scheme in which both the transmitting and receiving antennas are collocated (closely spaced) for coherent transmission and detection. The project will also include investigating transmit waveform design and in particular waveform correlation, sensor and sub-array

configurations, effects of multiplicative noise on signal-to-noise ratio and resulting image quality, and will develop appropriate SAR image reconstruction and GMTI detection algorithms.

4. **Automatic Identification and Mitigation of Unauthorized Information Leaking from Enterprise Networks**. A Phase II STTR contract was awarded to Secure Command, Inc., in partnership with George Mason University. The goal of this research effort is to develop a robust prototype of a transparent network proxy that can support both passive fingerprinting techniques and active content challenges that actively query VoIP requests with puzzles. The ultimate goal is to develop a prototype that is production ready to run for extended periods of time and support HTTP, VoIP, and other protocols as required, in different networked environments while meeting the stringent criteria for protecting DoD networks.

5. **Hybrid System Framework for Detecting, Classifying, and Mitigating Malicious Outbound Network Traffic Flows**. A Phase II contract was awarded to Milcord, LLC, with research participation from Dartmouth College. In Phase I of the project, the research team jointly researched and developed a software prototype that applies machine learning algorithms to contextual metadata, and entropy based sensors for the purpose of detecting data exfiltration on a computer network in real-time while accurately distinguishing between legitimate and anomalous behavior. Under the Phase II project, the team will build a full-scale flexible prototype that can be applied to not only known covert channels but also to any covert channel that is likely to sprout within the course of the project. The researchers will evaluate the performance of the developed system using live large scale network traffic data by implementing the developed algorithms on a state of the art parallel supercomputer for near real-time analysis, and on the emerging stream processing engines for real-time detection performance.

6. **System to Analyze Facial Features to Enable Operator Condition Tracking (AFFECT).** A Phase II STTR contract was awarded to Charles River Analytics, in partnership with Professor Mark Frank at the University of Buffalo. This project focuses on developing the Analyze Facial Features to Enable Operator Condition Tracking (AFFECT) system for the non-contact classification of stress, anxiety, uncertainty, and fatigue (SAUF) in interface applications. The AFFECT system will combine classification techniques with a multi-dimensional, temporal data model of novel visible and thermal features to enable automatic, non-invasive detection of SAUF conditions in a subject. The development of this technology will in turn enhance training, workflow, and overall effectiveness of analysts and warfighters.

7. **Trustworthy Execution of Security-Sensitive Code on Un-trusted Systems** A Phase II STTR contract was awarded to VDG, Inc. with research participation from Carnegie Mellon University. The objective of this project is to design, analyze, implement, and evaluate a system that enables user-verifiable execution of code on untrusted computer systems in the presence of malware. Based on a secure hypervisor that provides and enforces strong security even when the operating system and applications contain security vulnerabilities, the system protects security sensitive code and data on untrusted commodity platforms from malware (*e.g.*, kernel-level rootkits). Two specific implementations will be made to demonstrate the effectiveness of the proposed system: a secure browser environment and a general application. Ultimately this new secure hypervisor will provide a safe execution environment for security-sensitive code modules without trusting the OS or the application that invokes the code module.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

No new starts were initiated in FY10.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Computing Sciences Division

managed seven new DURIP projects totaling $1.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to uncover the fundamental principles of robust of resilient wireless communication systems and to develop novel computer vision systems that mimic natural human visions.

I. Congressionally-directed Cyber-security Laboratory (CyLab) at Carnegie Mellon University (CMU)

The CMU CyLab combines the efforts of more than 40 researchers and 100 students from the College of Engineering, the School of Computer Science and H. John Heinz III School of Public Policy and the CERT Coordination Center. In the area of information assurance, current research is carried out under six themes: (i) Resilient and Self-Healing Systems, (ii) User Authentication and Access Control, (iii) Software Measurement and Assurance, (iv) Information Privacy, (v) Threat Prediction Modeling, and (vi) Business and Economics of Information Security. The CMU CyLab is working closely with ARO to discover breakthrough technologies that can secure and protect the computing and communication capabilities of the Army. Successful results from these research efforts will contribute to the development of a highly assured, efficient, and survivable information system for future combat forces.

J. Congressionally-directed Cyber-Threat Analytics (Cyber-TA) Research Consortium

The mission of the consortium is to explore and develop advanced capabilities to defend against large-scale network threats and to create new technologies to enable next-generation privacy-preserving digital threat analysis centers. Currently, the consortium is led by SRI International, a non-profit research institute. The consortium consists of nine universities, two non-profit research organizations, and three small businesses, with more than 20 researchers participating. The project thrusts focus on: (i) privacy-preserving schemes for internet-scale collaborative sharing of sensitive information and security log content, (ii) real-time Malware-focused alert correlation analyses, including contributor-side correlation applications with repository-side reassembly, and (iii) new threat-warning dissemination schemes to rapidly inform large-scale multi-enterprise environments of new attack patterns and malware mitigation strategies that take advantage of the collaborative data correlation analysis. The researchers have already developed cutting-edge technologies and new tools that have been deployed to protect DoD information infra-structure. Most recently they developed effective analysis tools and counter-measures against the latest wave of intelligent attacks, such as the Conficker computer worm.

K. Congressionally-directed Secure Open Source Institute (SOSI)

A national center was established at North Carolina State University in FY08 to carry out research and develop trustworthy open source systems, techniques, and tools. The goal of the center is to develop a new computing architecture called a Secure Virtual Computing Architecture (SVCA) that will provide on-demand and secure delivery of a generalized computing environment (from a plain desktop, to classroom sized group of users, to cluster of servers, to high-performance computing) to an authenticated and authorized user located anywhere in the world. The system will be engineered such that there is mutual trust between the system, user data, and the users themselves. Several industry partners (*e.g.*, Red Hat, IBM, Cisco, Nortel) are collaborating with researchers to facilitate technology transfers and conduct joint research. The researchers at the center have recently focused on developing cost effective security solutions for virtual computing and cloud computing.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Computing Sciences Division.

A. Analysis of High-dimensional Signals using the Sparse Matrix Transform (SMT)

Professor Charles Bouman, Purdue University, Single Investigator Award

As sensing systems become more complex, the dimensionality and quantity of data grow rapidly. In particular, high resolution imaging systems, hyperspectral sensors, and large sensor networks represent sources of data that pose ever-increasing challenges to current data analysis methods. This research project focuses on developing a novel approach to sparse matrix transformations (SMT) for estimating, representing, and analyzing the correlation in high-dimensional signals using a sparse representation of the covariance.

Many existing pattern-recognition methods, such as principal components analysis (PCA) and linear discriminant analysis (LDA) are used to identifying unique regions in images for use in facial recognition. SMT is a new class of transformations that is a generalization of both the fast Fourier transform and orthonormal wavelet transform, but allows for adaptive processing of non-stationary signal. The PI has successfully designed SMT algorithms by performing a sequence of pair-wise coordinate transformations known as Given's rotations. By constraining the number of rotations, the algorithms constrain the space of de-correlating transforms to a non-linear manifold thereby allowing the full set of eigenvalues and eigenvectors of the covariance matrix to be estimated even when the number of observations is less than the dimension of the observations. Furthermore, SMT has been applied to graphical structures, thereby making it applicable to problems such as face recognition (i.e., image detection) and signal detection on sensor networks. The investigators found that SMT is superior to LDA analysis when the number of training samples is limited, demonstrating an improvement in classification accuracy (see FIGURE 2). This new fundamental approach to pattern recognition provides new methods and algorithms for sparse signal processing in a wide range of applications, including surveillance, biometrics, and robotics.

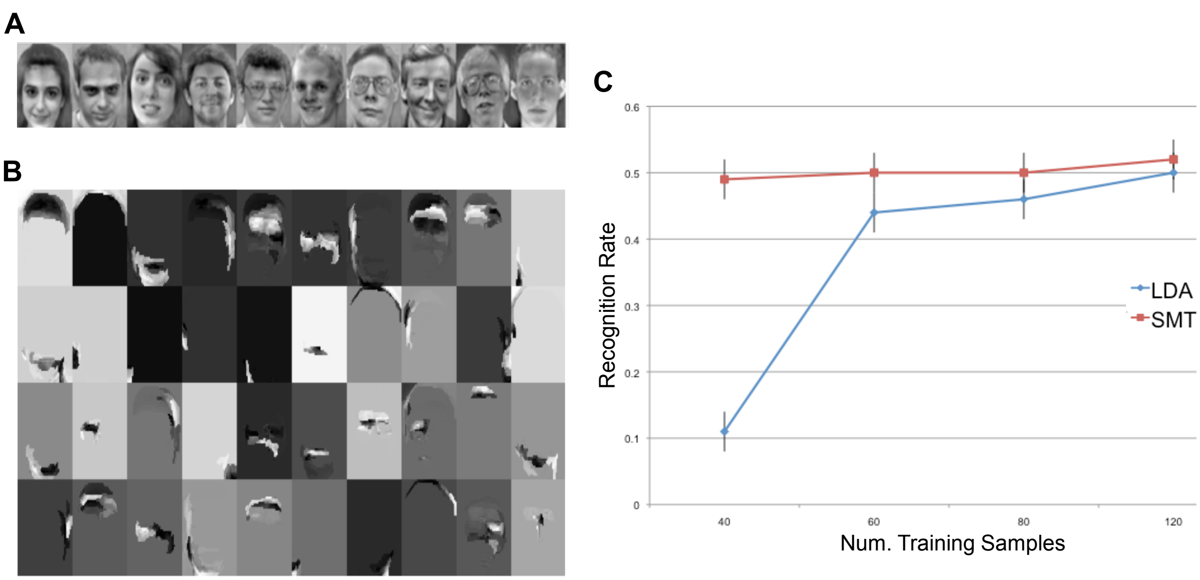

FIGURE 2

The SMT method can be used for eigenimage analysis. (A) Facial images from the Olivetti Research Laboratory (ORL) database (a commonly-accessed database for testing facial analysis methods) were analyzed using the SMT versus LDA methods. (B) The SMT method was employed to produce a full spectrum of eigenfaces, with each eigenface capturing local features resembling anatomical parts as identifiable components. (C) Relative to LDA, the SMT algorithm has higher recognition rates with lower numbers of training samples and reduced complexity for on-line computations.

B. Collaborative and Persistent Target Tracking and Acquisition
Professor Ying Wu, Northwestern University, Single Investigator Award

Visual information is subject to large uncertainties and ambiguities induced by factors such as cluttered and distractive backgrounds, illumination changes, visual occlusion, and low image quality. All these issues have impeded the development of effective and robust methods for persistent target tracking and acquisition in unconstrained environments. The goal of this effort is to discover new theory and computational methods that bridge computational sensing and some aspects in human perception of visual dynamics by creating multi-level synergy among various modalities and sensors.

This project is exploring how the spatial contexts can help construct accurate and robust matching. The PI has discovered a new approach called context flow, in which the spatial context is represented by the posterior density of the associated feature class and is used to constrain motion estimation for target tracking. Each individual context gives a linear contextual flow constraint to the motion so that the motion can be estimated in an over-determined contextual system. This approach is particularly useful for mitigating the challenges in video-based tracking of small targets in a dense environment of clutter in which the image resolution of the target is too low to provide reliable information for matching, and in turn, the clutter generates a large number of false positive matches and distractions. As the spatial contexts provide extra constraints in target matching and additional verification in data association, taking the advantage of the contextual information can improve the robustness of target tracking.

The PI has designed a new method of context-aware tracking for small targets, in which a set of motion-correlated auxiliary objects are automatically discovered on-the-fly, and each generates a specific spatial context of the target and leads to a contextual constraint to the target motion. Laboratory testing has indicated significantly improved performance in visual tracking. The research has high potential of leading to enhanced tracking capabilities for several important military applications, including persistent surveillance and robotics.

C. New Trusted Virtual Computing
Professor Peng Ning, North Carolina State University (NCSU), MURI Award

Hypervisors have been assumed to be trusted in many virtualization-based security services; however, there has been insufficient research focusing on their protection. The increasing complexity and the growing code size of existing hypervisors (*e.g.*, Xen) make it very difficult to avoid having vulnerabilities that could be exploited by attacks. Thus, it is critical to protect hypervisor integrity to ensure the trustworthiness of sensor data collected from the host, which will be used to support human centric cyber situational awareness.

NCSU researchers have developed HyperSentry, a novel framework to measure the integrity of a running hypervisor and to ensure that the hypervisor-based host sensors have high integrity and produce trustworthy raw data for cyber situational awareness (see FIGURE 3).

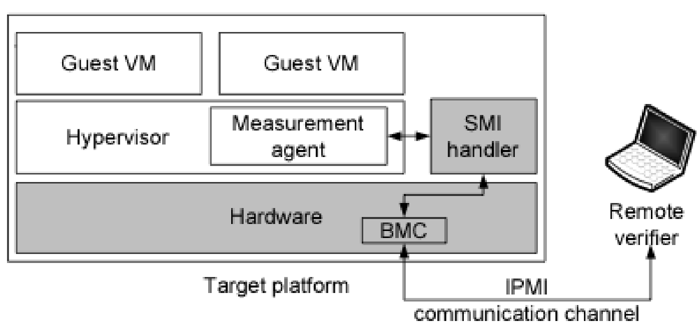

FIGURE 3

HyperSentry, a novel framework to measure the integrity of a running Virtual Machine (VM). Within this framework, the Intelligent Platform Management Interface (IPMI) manages the interface between the remote verifier and the target platform. (SMI: System Management Interrupt; BMC: Baseboard Management Controller)

HyperSentry is triggered by an out-of-band communication channel established with the Intelligent Platform Management Interface (IPMI). Despite the hypervisor's full control over the software system, HyperSentry uses

a novel technique to guarantee the stealth of this channel, which is critical in ensuring that a compromised hypervisor does not have the chance to hide the attack traces. Moreover, HyperSentry uses the System Management Mode (SMM) to protect its base code and critical data. It uses a set of novel techniques to overcome the SMM's limitation in retrieving the information required for integrity measurement. In particular, HyperSentry provides an integrity measurement agent with (i) the same contextual information available to the hypervisor, (ii) completely protected execution, and (iii) attestation to its output. To evaluate HyperSentry, a prototype of the framework along with an integrity measurement agent for the Xen hypervisor has been developed. Evaluation results demonstrate that HyperSentry is a low-overhead practical solution for real-world systems. This project is a collaboration with the IBM Research Center and the IBM System Group.

D. New methods for Detection and Response to Web Spam Attacks

Professors Pang-Ning Tan and Anil K Jain, Michigan State University (MSU), Single Investigator Award

As online social media applications continue to gain in popularity, concerns about the rapid proliferation of Web spam has grown in recent years. New social media applications allow spammers to submit links anonymously, diverting unsuspected users to spam Web sites. Unlike search engine spam, Web spam from social bookmarking and social news aggregator Web sites are potentially damaging because it may direct users to malicious Web sites that compromise browser security.

Professors Tan and Jain at MSU have investigated and created a novel co-classification framework to simultaneously detect Web spam and spammers in social media Web sites based on their content and link-based features. Based on the two assumptions that Spam URLs are more likely to be posted by spammers than non-spammers and that spammers are more likely to link to other spammers than to non-spammers, MSU researchers formalized these assumptions as graph regularization constraints and developed a co-classification algorithm to learn a pair of classifiers that simultaneously detect Web spam and spammers at a social media Web site. Using data from two real-world applications, the proposed co-classification framework has demonstrated to be more effective than other learning schemes that classify the Web spam and spammers independently. The framework can be easily extended to combine information from multiple social media Web sites, for better classification accuracy.

E. Real-Time LINUX for Multi-core Platforms

Professor James Anderson, University of North Carolina, Chapel Hill, Single Investigator Award

Thermal and power problems impose limits on the performance that chips with a single processing unit can deliver. Multi-core architectures (or chip multiprocessors), which include multiple processing units on a single chip, are being widely touted as a way to circumvent this impediment. The objective of this project is to obtain a fully-functional operating system (OS) for supporting real-time workloads on multi-core platforms.

This research effort achieved significant theoretical accomplishments this year by establishing tardiness bounds for soft real-time systems. New proof that task execution times can be specified stochastically and tardiness bounded in expectation leads to significant performance enhancement on soft-real-time applications that are typically provisioned assuming average-case, rather than worst-case, execution times. Professor James Anderson and collaborator Professor Sanjoy Baruah have improved prior tardiness analysis by developing new analysis that allows lower tardiness bounds to be established. These theoretical results have important practical implications as they can be applied to systems where tasks may suspend due to I/O operations, have precedence constraints (expressible using directed acyclic task graphs), and have non-preemptive sections. Real-time multi-core system are of increasing importance to the Army and DoD as more and more of these multi-core platforms are deployed and incorporated into Army and DoD systems.

F. Visualization of High Order Finite Element Methods

Professor Robert Kirby, University of Utah, Single Investigator Award

High-order finite element methods (also known as spectral/hp element methods) using either the continuous Galerkin (CG) or discontinuous Galerkin (DG) formulation, have reached a level of sophistication such that they are now commonly applied to a diverse set of real-life engineering problems. However, the visualizations of

high-order finite element results do not respect a priori knowledge of how the data were produced and do not provide a quantification of the visual error produced. This may undermine the scientific process because isolating where errors and assumptions are introduced into the process is critical. The goals of this effort are to define, investigate, and address the technical obstacles inherent in visualization of data derived from high-order numerical methods and to develop algorithms and software solutions that can be employed by the high-order simulation community.

The team has continued their efforts to understand how one accomplishes verification of isosurface extraction techniques. In FY09, the team successfully examined how well isosurface extraction techniques respect the topological features of extracted isosurfaces. They found that most, if not all, commonly used techniques do not respect topological invariants of isosurfaces. Based upon their studies they were able to propose and implement a new isosurface algorithm, which respects the topology of the underlying representation (see FIGURE 4). In addition, the team also continued work on the ray-tracing of isosurfaces of computational results that come from isogeometric analysis. Since isogeometric analysis is being heralded as the next big push within high-order finite elements for mechanics, it is important to consider the advantages and constraints of attempting to visualize this new type of high-order finite element data. The research results are of great importance to the Army since visualization is used by Army scientists as a key enabling technology for scientific insight. In particular, visualization is the main Army area of computational science concerned with the presentation of potentially huge quantities of data to aid cognition, hypothesis building and reasoning. If visualization is the lens through which Army scientists often view modeling and discretization interactions, then visualization must be explicitly considered as part of the validation and verification process in concert with the simulation technology.

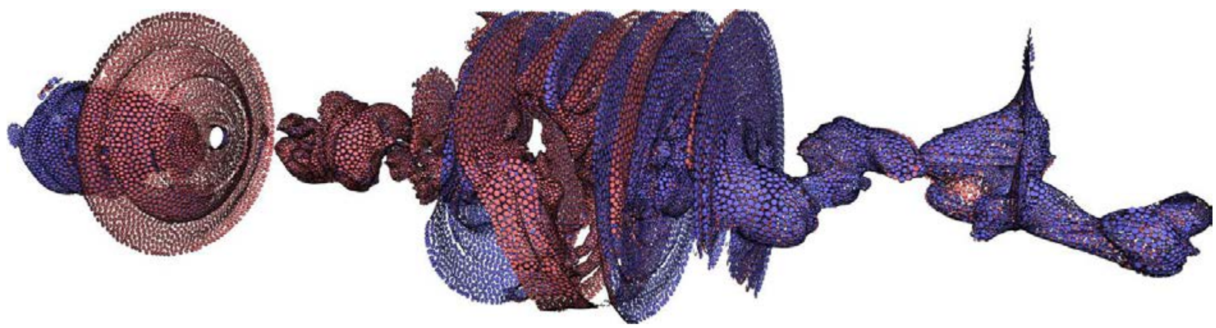

FIGURE 4

Isosurface of a finite element fluid simulation pressure field sampled with a particle system.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. New Multi-model Biometric Fusion System

Investigator: John Schneider, Ultra-scan Corp., SBIR Contract
Recipient: DoD Biometrics Identity Management Agency (BIMA)

Ultra-scan researchers have recently developed a new interoperable biometric platform that provides real-time multimodal fusion for human identification and verification. The platform incorporates an optimal fusion algorithm that the team has adopted and theoretically proven that has the capability to work with multiple biometric systems and with very large databases. A receiver operating characteristic (ROC) curve of the fusion algorithm demonstrates that the fusion system has a much better accuracy over the traditional single modality system (see FIGURE 5).

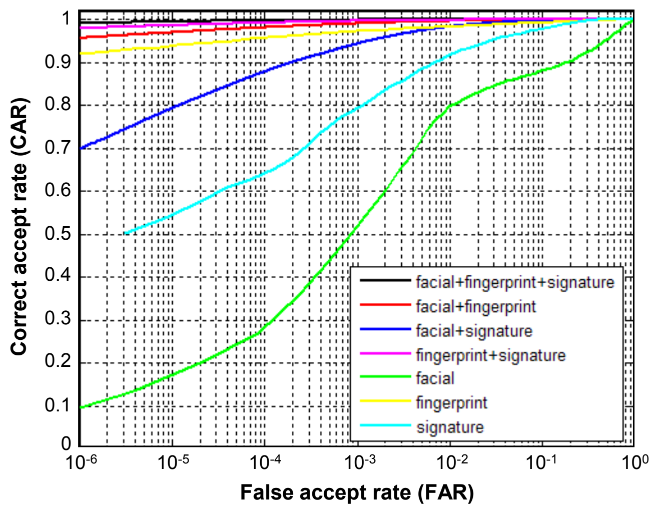

FIGURE 5

Receiver operating characteristic (ROC) curve of the fusion algorithm. The multi-modal system's ROC curve demonstrates the effectiveness of multi-modal fusion system, which greatly enhances human identification and verification accuracy.

This optimal multi-modal biometric fusion system targets a technology readiness level (TRL) of 7. A successful transition and integration of this new capability will greatly enhance accuracy and efficiency of DoD biometric operations at the Biometrics Identity Management Agency (BIMA; formerly the Biometrics Task Force). Validation and testing of the platform is being carried out with BIMA collaboration. A prototype system was installed at BIMA in late FY09 for field trials and testing.

B. Multimodal Information Fusion and pattern Classification via Symbolic Dynamic Analysis

Investigator: Shashi Phoha, Pennsylvania State University, MURI Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

The goal of this project is to create new theory and methods for reliable data/information fusion in heterogeneous sensor networks that can simultaneously achieve low probability of false detection and high probability of successful detection of event patterns. To that end, the researcher has created a novel language theoretic framework, the probabilistic finite state automata (PFSA), to represent and fuse heterogeneous sensor data. This framework allows efficient representation of multi-modal sensor data that retains all the semantic information in the sensor data while discarding redundant data, thereby leading to significant sensor data compression. The

computational algorithms for multimodal information fusion derived from the PFSA framework are being applied and tested using operational data at ARL-SEDD, toward developing advanced capabilities for human/vehicle event detection and classification in a heterogeneous sensor network.

C. Multi-Resolution Algorithms for Real-time Visualization, Reasoning and Interaction

Investigator: Ming Lin, University of North Carolina, Chapel Hill (UNC-CH), Single Investigator Award
Recipient: U.S. Army Cold Regions Research and Engineering Laboratory (CRREL)

Professor Ming Lin and Professor Dinesh Manocha, both at UNC-CH, initiated a collaboration in FY10 with Drs. Keith Wilson and D. Stephen Ketcham at CRREL in New Hampshire. The goal of this research is to apply the efficient representations and algorithms developed for real-time visual rendering based on ray tracing and multi-resolution representations to acoustic simulation of complex environments. The technology developed at UNC-CH is being transitioned to researchers at CRREL and will be applied to many Army scenarios and applications. The CRREL scientists are also interested in developing new and fast algorithms for sound field computations for situations, where neither prior low-frequency nor high-frequency methods are appropriate. In this context, new hybrid methods developed at UNC-CH will be very useful (*e.g.*, 50-500 Hz atmospheric acoustics) for when there is some randomness in the propagation but not enough that the problem can be modeled using a random scattering theory. The Army needs new set of algorithms for such cases. Moreover, the resulting technology will also be applicable to other direct battlefield applications, including battle planning on the operational scale of a brigade combat team, real-time source localization and camera pointing from acoustic arrays on aerostats, and dynamic routing of surveillance aircraft such as helicopters and UAVs to minimize audibility.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Novel Interactive Visibility Techniques

Professor Christopher Wyman, University of Iowa

Professor Wyman is conducting research funded through an STIR project with the goal of exploring novel visibility techniques for defense simulations that are less computationally burdensome than existing techniques, yet have associated error estimates to provide confidence levels for the results. Visibility algorithms play an important role in virtually all simulation environments, including Army applications such as training simulators and virtual ballistics computations, and civilian applications such as video games and computer generated movies. Unfortunately, naive visibility evaluation has order $O(n^4)$ complexity, scaling poorly to the geometric complexity necessary in many defense applications. His approach is to interactively identify regions with potential visibility problems as opposed to simply visualizing offline results which may waste computational effort in unimportant areas. This analysis will be done in screen-space, on a per-pixel basis, rather than the traditional world-space coordinates, which avoids expensive updates to global data structures focusing on changes that affect currently visualized data. The choice of metric is critical to properly identifying regions of interest and for developing error estimates. Three metrics will be investigated relying on three different, well-understood mathematical and geometric properties: conservative rasterization, randomized sampling, and Plucker coordinates. Selective refinement techniques will also be applied to adaptively improve simulation fidelity.

It is anticipated that in FY11, the researcher will develop and test new techniques for the interactive identification of regions with potential visibility discontinuities, develop a quantification method for the error, and ultimately, a preferential refinement of areas with the largest errors. This research outcome will lead to a significant reduction in computational effort for important Army simulations, such as virtual ballistics where simulations to fully test materiel performance under a variety of adverse conditions and from all possible angles often take a significant amount of time and computational resources.

B. Visual Information Theory and Visual Representations for Achieving Provable Bounds in Vision-Based Control and Decision

Professor Stefano Soatto, University of California, Los Angeles (UCLA)

A fundamental contribution by Shannon to the theory and practice of communications is Rate-Distortion Theory. This theory quantifies the expected probability of error in transmitting a binary symbol across a channel (distortion) with the "cost" of transmission (rate). The Rate-Distortion Theory has guided the development of compression algorithms for data storage and transmission. For any given desired probability of error, the theory specifies the minimum capacity that the channel must be designed for in order to attain such a probability of error. A similar theory describing cost-performance tradeoffs for visual decision tasks would be highly desirable, and it would enable characterizing the performance in detection, localization, recognition and categorization tasks, autonomous guidance, targeting and other applications of interest to DoD.

Recent work in Professor Soatto's laboratory has pointed the way to a generalization of Shannon's Rate-Distortion Theory for vision-based decision tasks. The key observation is that the "cost" that trades off performance in a vision-based decision task is not the number of pixels or the computational complexity, but the control authority that the sensing platform can exercise, in terms of the subset of physical space that is covered by the reachable set of the controller actuating the platform. This means that in order to guarantee a given probability of error, processing passively gathered data is insufficient. Instead the sensing platform must be controlled to gather additional data if the error bound is not met by the existing data.

It is anticipated that Professor Soatto will establish a theoretical foundation for characterizing the "perception-control" tradeoff, that describes the expected probability of error in a basic detection task (binary classification describing the presence/absence of a given target in a scene) as a function of the volume of the reachable space and the energy expended by the controller. The theory will indicate (i) what probability of error can be guaranteed for a given amount of resources (mobility, energy and resolution), and (ii) what kind of data must be gathered (i.e. what control sequences must be actuated) in order to attain a given probability of error where the available data is insufficient. Soatto's group is working simultaneously at deriving an analytical characterization of such a tradeoff, as well as empirically evaluating this tradeoff for simple simulated one-dimensional robots moving in a flat two-dimensional space. A key barrier to enabling such a development is the availability of efficient algorithms to detect occlusions in images and video. This problem, long thought to be a strongly non-linear, non-convex infinite-dimensional optimization problem, has been recently shown to be convex so a global optimal solution exists and can be expected with efficient numerical schemes.

C. Enhancing the Security of Wireless Systems through Opportunistic Secret Communication
Professor Wade Trappe and Professor Roy Yates, Rutgers University

Securing wireless and mobile communications has been a challenge in large part due to the broadcast nature of the wireless medium, where eavesdropping and adversarial transmissions can be easily accomplished. Conventional ways to secure wireless communication are through confidentiality services and/or authentication services, with the support of key establishment. Recent research has shown that the wireless medium itself can serve as a mechanism to share secrets for key establishment by exploiting the variability and dimensionality associated with wireless propagation.

A new initiative at the Rutgers University Wireless Information Network Laboratory (WINLAB) is investigating and examining the issues of securely sharing bits through wireless channels. This project focuses on examining the challenges of information-theoretic secret communication that utilizes the unique capacity and diversity enhancing advantages of the wireless medium to improve secret communication rates. Underlying the effort is the philosophy that improved secrecy can be achieved, even when the adversarial channel is better than the legitimate channel, because of the variations inherent in the wireless channels. The technical objective is to develop opportunistic methods to exploit these variations while simultaneously addressing the need for efficient key dissemination.

In FY11, it is anticipated that the researchers will carry out experiments using software defined radio platforms for validation and verification of theoretical analysis and models and to ensure the relevance of the underlying research to practical wireless systems. These studies will include investigations of secrecy capacities in orthogonal frequency-division multiplexing (OFDM), time-varying flat fading, time invariant multiple-input and multiple-output (MIMO) and time-varying MIMO channels for three distinct adversarial models characterized by the types of channel state information (CSI) available to the adversary. Ultimately, this research will lead to the establishment of the underlying theory behind secrecy dissemination methods for wireless systems and will build the foundation of physical layer-enhanced security in more general wireless network scenarios.

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CHAPTER 5: ELECTRONICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Electronics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to gain new fundamental knowledge of electro-magnetic, photonic, and acoustic devices, systems, and phenomena. More specifically, the Division aims to promote basic research studies to discover and control the relationship of nanostructure and heterostructure designs on charge transport and carrier recombination dynamics, to understand and improve the stimulus-response properties of electronic materials/structures, to leverage nanotechnology for enhanced electronic properties, to comprehend and mitigate distortion and noise, and to explore ultra-fast, solid state mechanisms and concepts. The results of these research efforts will stimulate future studies and help keep the U.S. at the forefront of research in electronics by revealing new pathways for the design and fabrication of novel electronic structures that have properties that cannot be realized with current technology.

2. Potential Applications. Electronics research is relevant to nearly all Army systems; therefore, research under this program provides the underlying science to a wide variety of developmental efforts and contributes to the solution of technology related problems throughout the full spectrum of the Army's "System of Systems." Research in electronics can be divided into five areas: (i) multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas, (ii) ubiquitous communications for multimode and secure communications in all situations including high data rates, transmission over long distances and complex terrain paths, as well as problems associated with short range networked systems, (iii) intelligent information technology that enhances the creation and processing of information, (iv) optoelectronic warfare, which involves the use of electromagnetic (EM) radiation from radio frequency (RF) to ultraviolet (UV), to interrogate, disrupt, and defeat hostile electronic and threat systems, and (v) power electronics for electronic circuits and components that require less power and/or operate in extreme conditions.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Electronics Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research, the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). Moreover, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, sensing is a research element of all ARO Divisions, and the Electronics Division serves as the focal point for ARO sensing research. Specific interactions include joint projects with the Physics Division that promote research for physics-based understanding of semiconductor materials, non-reciprocal materials and devices, propagation effects, and stimulus response effects in condensed matter. The Electronics Division also coordinates efforts with the Materials Science Division to pursue the design and characterization of new materials and structures, the evaluation of electrical properties, and the study of electronic processes at the molecular level. This Division complements its research initiatives in the Chemical Sciences Division to include research to understand how chemical changes and chemical structures influence electrical, magnetic, and optical

properties and investigations of high frequency spectroscopic techniques for use in chemical defense, especially explosive detection. The Life Sciences Division's Program Areas also interface with electronics research in areas of biological detection as well as interfacing to biological organisms. Lastly, creating computational methods and models for target recognition and understanding nano-molecular structures and carrier transport shared research goals between the Electronics and Mathematical Sciences Divisions.

B. Program Areas

To meet the long-term program goals described in the previous section, the Electronics Division engages in the identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within four Program Areas: (i) Solid State and High Frequency Electronics, (ii) Electromagnetics, Microwaves, and Power, (iii) Optoelectronics, and (iv) Sensors and Detectors. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Solid State and High Frequency Electronics. The goal of this Program Area is to conduct research into quantum phenomena, internally and externally induced perturbations, and novel transport and optical interaction effects in nano-scale electronic structures. This Program Area is divided into two research Thrusts: (i) Nanoelectronic Engineering Sciences, and (ii) Teraherz-frequency and Ultra-fast Electronics. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. This Program Area includes research efforts in quantum-confined structures, nonequilibrium and dissipative electron processes in low-dimensional device structures, novel contact and interconnects to nanoscale devices, physics and modeling of nanoscale devices and advanced synthetic materials, novel materials and heterostructures, device based upon mixed-mode principles, mixed technology (*e.g.*, photonics, acoustics and magnetics) systems, and heterogeneous (*i.e.*, different materials and device principles) systems. This research program will have a particular emphasis towards ultra-fast and terahertz frequency electronics and will include a strong component for sensing science at very high frequencies.

This Program Area's research efforts involving nano-devices and molecular-level electronics will address issues related to the design, modeling, fabrication, testing and characterization of novel electrically and magnetically-controlled electronic structures. This research will enable the development of novel materials, advance processing and fabrication science, the development and implementation of advanced physical modeling and simulation capabilities, and the identification of advanced electronic device concepts. These investigations will ultimately lead to improvements in the current limits on the functionality, power, speed (frequency) and power consumption of electronic components. This research is a key enabler for many U.S. Army future electronic goals as it supports an array of capabilities in densely integrated nanoscale architectures for ultra-sensitive and high-discrimination sensing, high-speed, high-data-rate communications and signal processing, and enhanced high-frequency power, efficiency, and sensitivity.

2. Electromagnetics, Microwaves, and Power. The goal of this Program Area is carry out basic research leading to the creation of a transmit/receive system that will receive and demodulate any electromagnetic signal from any direction, modulate and transmit any electromagnetic signal in any direction, reconfigure to implement a variety of radio and sensor functions, adapt to the ambient environment, and respond to changing requirements. This Program Area is divided into three research Thrusts: (i) Electromagnetics and Antennas, (ii) RF Circuit Integration, and (iii) Power Efficiency and Control. These Thrust areas guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. Research efforts within these Thrusts include studies of the generation, transmission, and reception of high frequency microwave and millimeter wave radiation, as well as specific technical problems at high frequency (HF), very high frequency (VHF), and ultra-high frequencies (UHF). Research efforts within these Thrusts include studies of the coupling of electromagnetic (EM) radiation into and out of complex structures, active and passive antennas, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques that advance mixed-signal design to the state of current digital design.

The research efforts within this Program Area may lead to the discovery of novel active and passive devices and components with improved dynamic range, linearity, bandwidth, and loss performance. This includes

improvements which have the greatest system leverage in reducing radio and radar power requirements, battery size, and system size. Physical constraints imposed by 2D mixed-signal circuit integration and parasitic power loss in passive components are being addressed and novel approaches to circuit integration, such as use of 3D, plug and play circuit integration are being explored. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

3. Optoelectronics. The goal of this Program Area is to discover and control novel nanostructure and heterostructure designs for the generation, guidance, and control of optical/infrared signals in both semiconductor and dielectric materials. The research in this program may enable the design and fabrication of new optoelectronic devices that give the Soldier high-data-rate optical networks including free space/integrated data links, improved IR countermeasures, and advanced 3D imaging. This program has three Thrust areas: (i) High Speed Lasers and Interconnects, (ii) Ultraviolet and Visible Photonics, and (iii) Mid-infrared Lasers. The research topics involve efforts to overcome slow spontaneous lifetimes and gain dynamics, low carrier injection efficiency, poor thermal management, and device size mismatches. Novel light emitting structures based on III-V compounds, wide bandgap II-VI materials, rare-earth doped dielectrics, and silicon nanostructures are being investigated along with advanced fabrication and characterization techniques. Nanotechnology is exploited to allow interfacing of optoelectronic devices with electronic processors for full utilization of available bandwidth. Electro-optic components are being studied for use in guided wave data links for interconnections and optoelectronic integration, which are all requirements for high speed full situational awareness. In addition, emitters and architectures for novel display and processing of battlefield imagery are also important to this program.

4. Sensors and Detectors. The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Infrared Detectors and (ii) Non-imaging Sensing. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. The scientific objective of the Infrared Detector Thrust area is to understand and control the stimulus and response of infrared materials and devices. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as devices made of amorphous materials. An important element in this Thrust area is the reduction of performance limiting defects in semiconductor material and structures through lattice matching and other methods. Development of novel characterization techniques is also explored to determine the fundamental issues behind carrier transport, lifetimes, and noise. Research in this Thrust area includes both high performance detector materials and structures and uncooled, low cost, detector materials and structures. The Non-Imaging Sensing Thrust strives to uncover the underlying relationships behind signature phenomenology and use it to guide sensor development and decision techniques. Non-Imaging sensing modalities include acoustic, magnetic, infrasound, and "passive" environmental signals such as radio or TV broadcasts. Efforts in the this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division in FY10 were $48.7 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $4.8 million. The Department of Defense Multi-disciplinary University Research Initiative (MURI), Defense University Research Instrumentation Program (DURIP) provided an additional $4.8 million to programs managed by the Electronics Division. The Division also managed $25.4 million of Defense Advanced Research Projects Agency (DARPA) programs, and $5.8 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $6.6 million for awards in FY10. Finally, $1.3 million in FY10 was provided from other sources for use in the Presidential Early Career Award for Scientists and Engineers (PECASE) and the Historically Black Colleges and Universities (HBCU) outreach programs.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. National Radio Science Meeting (Boulder, CO; 5-9 January 2010). This open scientific meeting is sponsored by the U.S. National Committee of the International Union of Radio Science (USNC-URSI) and Dr. Dev Palmer of the ARO Electronics Division served as co-chair of the Plenary Session. The USNC-URSI is appointed by the National Research Council of The National Academies and represents U.S. radio scientists and engineers in the international community. Papers on any topic in radio communications; electromagnetic phenomena, remote sensing, and other radio science areas of interest are presented. The meeting provided an excellent snapshot of the state of radio science and a common ground for discussion of future basic research topics.

2. IEEE Radio and Wireless Symposium (New Orleans, LA; 10-14 January 2010). This symposium focused on the intersection between radio systems and wireless technology, which created a unique forum for engineers to discuss hardware design and system performance of the state-of-the-art wireless systems. Dr. Dev Palmer of the ARO Electronics Division served as session chair and judge of the Student Paper Competition. The symposium attracted engineers from academia, government, and industry from the U.S. and around the world. This year's meeting featured a technical track on Sensors and Sensor Networks, which is highly relevant to Army situational awareness and force protection.

3. 2010 Laser Applications to Chemical, Security and Environmental Analysis (LACSEA) Conference (San Diego, CA; 31 January - 3 February). This interdisciplinary meeting focused on recent advances in analytical laser spectroscopy, including the development of new laser-analytical principles and new components, systems and applications. Dr. Dwight Woolard of the ARO Electronics Division was the co-technical organizer of the conference. Contemporary scientific topics were highlighted in areas such as: (i) new laser, optical, and spectroscopic science for analytical sensing, (ii) new fundamental spectro-analytical principles and techniques, including nonlinear and ultra fast spectroscopy and analytical use of optical frequency combs, (iii) new laser light sources, optical components and detectors for analytical systems from the VUV, UV, to the FIR and THz spectral range, (iv) improved data retrieval techniques in laser spectroscopic analysis, (v) new laser analytical instrumentation including, optical and micro-optical laser-based systems for chemical analysis and monitoring, laser analytical lab-on-chip systems, and distributed laser optical sensor networks, and (vi) innovative analytical applications of optical methods.

4. IEEE International Vacuum Electronics Conference (Monterey, CA; 16-20 May 2010). This conference focused on the broad spectrum of scientific issues and applications that drive current directions in vacuum electronics research. Engineers from academia, government, and industry attended the technical presentations, which spanned the range from UHF to THz frequencies and presented current work in theory and computational tool development, active and passive components, systems, and supporting technologies. Vacuum electron devices such as microwave power tubes are a critical component for high-power, high-frequency radar and communication systems. These systems fulfill key roles in command, control, communications, computing, intelligence, surveillance, and reconnaissance (C4ISR) and situational awareness, and enhance lethality through target detection, identification, tracking, and fire control, enhance mobility through all-weather navigation, and enhance survivability through threat detection and identification. The recent coupling of micromachining techniques with vacuum electronics has a high potential impact on military submillimeter-wave communications, ECM, and radar systems, and is directly responsive to future Army needs in C4ISR and mobile wireless communications. Dr. Dev Palmer of the ARO Electronics Division was a member of the organizing committee and served as session chair.

5. 2010 International Symposium on Spectral Sensing Research (Springfield, MO; 21-24 June). The goal of this bi-annual meeting was the creation of new technology-program oriented networks that serve to accelerate the key research and development efforts that underpin the leading spectroscopic-based early-warning sensor capabilities. To accomplish these goals, this symposium was strategically coordinated and partnered with the 2010 Joint Chemical Biological Radiological and Nuclear (CBRN) Conference and Exhibition at nearby Fort Leonard Wood to achieve a simultaneous enhancement of the two meetings in terms of their collective connections to: (i) newly emerging and innovative scientific and technological opportunities, and (ii) existing defense, protection and response technologies and doctrines, for addressing the serious threats posed by chemical, biological, radiological, nuclear and explosive (CBRNE) agents to the warfighter and civilian communities. Dr. Dwight Woolard of the ARO Electronics Division was the lead technical organizer of the symposium, which included several presentations by ARO-funded investigators.

6. Perspectives on Zinc Oxide Materials and Devices for Optoelectronics Workshop (Riverside, CA; 7-9 July 2010). This workshop was created in response to ARO to bring together the top performers and experts on zinc oxide and related wide-bandgap semiconductor oxide materials and devices related to optoelectronics to gather information and discuss forefront issues to advance the field. Dr. Mike Gerhold of the ARO Electronics Division was one of three co-chairs of the meeting. Three major sessions were held: (i) Homo-epitaxial and hetero-epitaxial ZnO-based thin films and alloys, (ii) p-type doping of ZnO thin films, alloys, and nanowires, and (iii) ZnO thin-film and nanowire light emitting diodes, laser diodes, and photodetectors. Panel sessions were held for each of the three sessions, and the resulting discussions led to better understanding of the state of substrates and epitaxial growth, p-type doping, and problems inhibiting strong electrically-injected lasers.

7. 2010 Lester Eastman Conference on High Performance Devices, (Troy, NY; 3-5 August 2010). The goal of this conference was to encourage active cross-fertilization in different technology areas, including high speed devices, power conversion, green emitter technology, infrared photonics, terahertz technology, and next generation devices. This conference brought together experts in academia, industry, and government laboratories to discuss new advances in materials and devices in each of these areas. Dr. Mike Gerhold of the ARO Electronics Division was a session chair and discussion leader for Next Generation Devices. One notable highlight in the Infrared Photonics session was the suggestion that the problem with the carrier lifetime in superlattice materials was not due to Shockley-Read-Hall recombination at the interfaces but rather phonon recombination. This needs further testing but, if correct, it will have important implications for Army programs on improving infrared detectors.

8. IEEE International Conference on Wireless Information Technology and Systems (Honolulu, HI; 28 August - 3 September 2010). This conference addressed research advances and recent development in the broad subject of wireless technology and its application in a wide variety of areas including, communications, national security, medical, transportations, and radar technologies. Scientists and engineers from academia, government, and industry gathered to participate in the program of technical sessions, workshops, and short courses, which included several special sessions organized by DoD engineers. Wireless information technology and systems form the technical underpinnings of network-centric warfare, networked communications, and electromagnetic sensing. This meeting had a special session on Army wireless communications that included presentations highlighting several ARO funded projects.

9. Joint OCS/ARL-ARO Audio Workshop on Advanced Technologies for Audio Collection and Transmission (Adelphi, MD; 9-10 September 2010). The goal of this workshop was to discuss fundamental concepts and new ideas in acoustic transduction and audio processing. The workshop was co-hosted by the ARL Sensors and Electron Devices Directorate (ARL-SEDD) Acoustic and EM Sensing Branch, and brought experts from the academic community together with scientists from the DoD and the intelligence community (IC) to review groundbreaking research in audio-related technologies, identify needs within DoD and the IC, and form recommendations for possible future basic research in acoustics and related fields. Dr. Dev Palmer of the ARO Electronics Division was co-chair of the workshop.

10. Antenna Applications Symposium at Allerton (Monticello, IL; 21-23 September 2010). The Antenna Applications Symposium and its predecessor, the Air Force Antenna Symposium, have for more than fifty years provided a unique forum for exchange of ideas and information about antenna design and development. The symposium brought together key researchers from all three military services, law enforcement, companies from the U.S. and abroad, and universities from across the country and around the world. Technology reviewed at the Allerton Symposium demonstrates the breadth of antenna applications, ranging from arrays for radar, communication, navigation and remote sensing, to innovative, multidisciplinary basic research concepts for antenna reconfigurability and multi-functionality, to numerical modeling techniques, all of which are highly relevant to Army missions in electromagnetic sensing and communications. Dr. Dev Palmer of the ARO Electronics Division served as the session chair and judge of the Student Paper Competition.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. Analyzing Human Electronic Signatures. This MURI began in FY04 and was granted to a team led by Professor William Rhodes at the Georgia Institute of Technology. The goal of this research is to understand of the phenomenology underlying the signatures generated by humans, the detection of those signatures using multiple sensor modalities, and the processing of those signatures to detect personnel.

In particular, the objectives are to understand the physics of signatures in traditionally difficult detection environments, identify sensor network constructs to record these signatures, and develop processing techniques (e.g., distributed processing) to exploit these signatures for personnel detection. The technical efforts focus on three sensor domains: seismic/acoustics, electro-optics, and radar. Seismic/acoustics technical efforts investigate use of passive and active sensing modes. Electro-optics research focuses on development of a multi-modal human signature and urban model, creation of motion-based detection algorithms, and development of techniques for detection in low pixel video sequences. Additional work focuses on exploiting motion capture data for human motion characterization and discrimination. Radar-based research focuses on improving autoregressive modeling approaches for gait detection and investigation of "passive" RF signals at local transmitter frequencies. The anticipated scientific advances will provide DoD with a significantly improved capability to detect personnel in scenarios of military interest. These include open and cluttered areas, urban environments, and caves and tunnels. This supports a critical military need for enhanced force protection and improved local situational awareness.

2. Standoff Inverse Analysis and Manipulation of Electronic Systems. Two efforts under this MURI topic began in FY05, with one effort led by Professor Michael Steer at North Carolina State University, and the second led by Professor Lawrence Carin at Duke University. These researchers are studying the interaction between electromagnetic fields and electronic circuits, with the ultimate goal being rapid and accurate extraction of system, functional, and device information from external stimulus and monitoring of electronic systems.

At the most basic level, the interaction between electromagnetic fields and electronic circuits is visualized as a radio signal being received through an antenna by a radio circuit. Most analytical models and system-level simulations are limited to this level of complexity, which gives accurate results only within the designed operating bandwidth of the system. In reality, electromagnetic fields can couple in and out of electronic circuits

in a variety of ways and through a variety of components, reducing performance and causing interference to other circuits. The MURI team is using sophisticated laboratory equipment to illuminate electronic circuits with EM signals over a wide range of frequencies using a variety of waveforms, and measure the signals re-radiated from the circuits. This approach has already revealed previously unknown phenomenology that has the potential for significantly improving the capability to identify, locate, and disrupt electronic devices at a distance.

3. Studying Stimulus-Response Properties of Uncooled Infrared Materials. This MURI began in FY06 and was awarded to a team led by Professor Mark Horn at Pennsylvania State University. The goal of this research is to gain knowledge of the physics and chemistry of uncooled infrared materials and quantify their fundamental and technological attributes and limitations.

The main focus of this research is on vanadium oxide (VO_x) and amorphous silicon germanium (a-$Si_{1-x}Ge_x$:H) materials but other novel materials are also being explored, such as the spinel family and zinc oxide (ZnO). A combination of theory, microanalysis, optical measurements, and feedback to growers is employed to unravel the mysteries of the structure, absorption mechanism, and transport properties in these largely disordered materials. An early surprise was the discovery of the face centered cubic structure for $VO_{1.8}$ that does not match the stoichiometry. This information plus conductivity measurements have led to a theory of charge transport wherein the mechanism changes from variable range hopping at low temperatures to nearest neighbor hopping at room temperature. It is hoped that this knowledge gained from this MURI can be used to make improvements in the materials to fully exploit their capability for uncooled infrared detector applications. Understanding at the molecular level of the dynamics of the materials will provide a quantitative fundamental base toward achieving the goal of an infrared camera for every Soldier in the field.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Solar-blind Photodetectors Based on Wide-bandgap Oxides. A Phase I SBIR contract was awarded to Tanner Research, Inc. to develop ZnBeO and ZnMgO alloy nanowire detectors in the 240-285 nm regime. Photoconductive gains of 10^8 were found in prior work on ZnO detectors at ~360 nm.

This project will use MOCVD for nanowire growth with ZnMgO and ZnBeO alloys. ZnO nanowires were previously developed for such a demonstration at 365 nm range with large photoconductive gains. Mg and Be will alloy into the ZnO and create a wider bandgap with similar gains for high signal to noise. One concern that was seen in previous ZnO nanowire work was the slow speed of the detectors. A special contact will be developed to reset the nanowires by draining stored charge and making the speed of the detector very fast and controllable. The proposed research will develop sensitive photodetectors in the 265-280 nm region of the UV optical spectrum, which is directly responsive to future Army needs non-line-of-sight communications, UV LED monitoring for water and surface disinfection/purification systems, and bio-agent threat warning systems.

2. Terahertz Emitter Based on Frequency Mixing in Microchip Solid-State Laser Cavity. Two Phase I SBIR contracts were awarded to ArkLight, Inc. and L. C. Pegasus Corp. to establish the foundation for the future development and demonstration of a compact, portable, widely-tunable, and narrowband terahertz (THz) emitter, based on frequency mixing of two lasing beams in a nonlinear crystal placed inside a dual-frequency solid-state laser cavity.

The field of THz spectroscopy holds promise in the identification and detection of biological and chemical species, but such applications have been impeded primarily by the lack of a miniature, portable, coherent, high-power, and widely-tunable THz source. These two Phase I SBIR efforts seek to significantly scale up the THz output powers by combining the advantages of intracavity frequency mixing and novel structures such as plasmonic metallic gratings. The ArkLight Inc. effort will investigate a revolutionary approach to THz generation based upon difference-frequency generation occurring within the cavity of a dual-wavelength Yb:YAG laser, and explore the most optimum nonlinear materials systems and document the tradeoffs regarding the choice of laser material and the nonlinear mixing material. The L.C. Pegasus Corp. effort will investigate difference frequency mixing based generation of terahertz frequency radiation where the frequencies to be mixed are generated in two KTP crystals pumped by a frequency-doubled Nd:YAG oscillator and the mixing will be

implemented within a waveguide with the input coupling achieved using a novel grating structure. This technology will significantly enhance the effectiveness of long-wavelength spectroscopy for use in chemical and biological detection applications.

3. ZnO Light Emitting Diodes (LEDs) and Laser Diodes. Two Phase I SBIR contracts were awarded to Cerment, Inc. and ZN Technology to develop useful LEDs and lasers across the visible spectrum into the UV. ZnO has inherent materials advantages over more developed GaN technology, which may make it a more efficient emitter at many useful wavelength for sensing, solid state lighting, and displays.

Cerment will advance the development of MgZnO-based LEDs and laser diodes through epitaxial growth of crystals on ZnO and other substrates, while ZN Technology will advance ZnO alloy based LED and laser diode technology based on the development of Zn(Mg,Cd)O alloys. P-type doping will also be studied and advances will be incorporated into devices. The proposed research will advance work in the field of ZnO LEDs and lasers in the UV-visible, which is directly responsive to future Army needs for solid state lighting, bioagent threat detection, water purification and surface decontamination. Laser diodes could also surpass GaN based diodes used in DVDs and optical data storage and be used for similar applications for increased data storage densities should deep-UV alloys and devices be possible (in the future).

The proposed research will advance the development of ZnO based light emitters, which is directly responsive to future Army needs for efficient UV-visible laser diodes and LEDs. Solid state lighting, bioagent threat detection, water purification, and multiple other uses are possible if ZnO based light emitters exceed competing technologies.

4. Alignment Tolerant Optical Interconnects for Missiles and Radar. Two SBIR Phase II Enhancement contracts were awarded to Ziva Corp. and UltraCommunications, Inc. to continue development of optical interconnect systems for missile and radar applications.

The goal of the Ziva Corp. contract is to enhance the functionality of the optical interconnect technology from simplex to full duplex and take the technology from a technology readiness level (TRL) 5 to TRL 6 at the end of this phase. More specifically, the research will further reduce the size of the transceiver modules to open up a larger number of applications and incorporate specific interfaces so that the technology can be demonstrated in specific military systems. The target systems include Medium Extended Area Defense System (MEADS) and other radar system applications. Fabricated modules will be tested first at Ziva to assure full functionality and then at Lockheed Martin. The goal will be to show a four channel multigigabit/s bidirectional (full duplex) link on one fiber, thereby showing a four times reduction in the number of fibers required. For the option period the approach will continue to develop specific interfaces to the MEADS platform. This project will benefit radar systems by reducing the size, weight, and cost of the cables connecting the radar to the CPU. Another benefit of the solution proposed here is that it is scalable in speed up to at least 40 Gb/s/channel.

The goal of the UltraCommunications contract is to move fiber-optics closer to high speed IC's, which improves processing speed, lowers power, and reduces the size and weight of comparable functions for military applications, such as missiles, where shock and high-g acceleration tolerance are critical. If successful, the UltraCommunications project will build and demonstrate a form-factor compatible fiber-optic link design for high-shock environments. This accomplishment would move the technology from TRL 3 to at least TRL 7, as it will at completion be in a form factor that a customer can use and test in a relevant shock environment.

These Phase II projects will significantly improve the real-time processing capability of missile/munitions systems thereby improving all flight control operations. Also, the increased bandwidth realized with fiber optic links will not only enable high speed digital communication, but also direct high speed analog and RF communication, which is currently not possible in the missile/munitions community.

5. Large-area Deep-UV LEDs Based on AlGaN Semiconductors. Two Phase II SBIR contracts were awarded to Nitek, Inc. and Sensor Electronic Technology (SET), Inc. to develop high power, large-area deep-UV LEDs at an emission wavelength of around 275 nm for various military and civilian applications, such as water purification and bio-warfare agent sensing.

The goal of the Nitek, Inc. effort is to create deep-UV LEDs, building on the double buffer approach using pulsed MOCVD growth for AlGaN multi-quantum-well (MQW) LEDs. Sensor Electronic Technology, Inc. will develop, prototype and start pilot production of a new class of high power deep ultraviolet (DUV) LED using

proprietary and patented processes that involve growth of low defect density, high Al-content thick template layers, by migration-enhanced metal organic chemical vapor deposition (MEMOCVD®) over patterned sapphire substrates. The proposed research will improve upon deep-UV LED technology using AlGaInN alloy heterostructures. This deep-UV LED technology is directly responsive to future Army needs for water purification, bio-agent sensing, surface sterilization, UV communications, as well as for a deep UV laser. Dual-use civilian applications include polymer curing and biomedical instruments.

6. Sensing and Communication Abilities of Biological Micro-electromechanical Systems (Bio-MEMs). Two Phase II Chemical and Biological Defense (CBD) SBIR contracts were awarded to OpCoast LLC and CFD Research Corp. to develop technologies that leverage the natural capabilities of insects to realize low cost sensor and communication networks.

Millions of years of evolution have endowed insects with abilities to communicate reliably over varying distances through the transmission and reception of characteristic chirping sounds. The spectral contents of insect calls can be quite complex, as evidenced by virtually unlimited patterns of repetition, sound timbre, inflection, and other characteristics. These spectral characteristics lend themselves to the possibility of low-bandwidth message passing by modulating the natural acoustic communication capabilities of insects. Recent developments in electro-biomechanical interfaces with insects are now able to form an exploitable organic platform.

The goal of these two Phase II SBIR efforts is to leverage and combine numerous properties of insects (e.g., calls, mobility) to achieve bio-inspired devices and systems that enable the efficient transfer of intelligent information. OpCoast LLC will focus on the development of the "OrthopterNets" concept (named after the insect order *Orthoptera,* which includes common crickets, katydids, and related calling insects) that utilizes a swarm of insects equipped with a capability to pass received messages to other similarly-equipped insects or receiver endpoints. OpCoast's primary path to OrthopterNets will be to leverage the natural acoustic sounds that are produce by "calling insects", such as crickets, by developing electro-mechanical actuators (and/or neural-muscular electrodes) and the required technology and communication protocols required for realizing message passing within insect swarms. The research focus of the contract with CFD Research Corp. is to generate electrical power from components in the fluids and create a research plan that develops and ultimately implements an insect platform capable of providing a neural stimulation system for modulating insect calling and an overall control system for monitoring chemical levels and translating the event to the communication methodology (*e.g.*, insect calling). Both of these efforts will contribute technologies for the development of completely integrated insect platform and would be useful for enhancing Soldier survivability by detecting dangerous threats (*e.g.*, chemical, biological, people) and assisting in search and rescue missions.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Coherent Beam Combining of Mid-IR Lasers. Two Phase I STTR programs were awarded to Intraband, LLC and Pranalytica, Inc. to study monolithic integration of quantum cascade lasers into coherently combined arrays scalable to 100 W or more.

The goal of the STTR contract led by Intraband, LLC is to design eight micron-emitting active-photonic-crystal (APC) quantum-cascade (QC) lasers using passive phase-locking in a monolithic structure in order to achieve multiwatt-range, diffraction-limited powers. The contract led by Pranalytica, Inc. will selectively overgrow an InGaAs waveguide core and an InP cladding between the antiguide array elements with minimal leakage current and a surface morphology designed for epi-down mounting. The anticipated benefits from developing the proposed eight micron-emitting devices stem from the over ten-fold increase in average power, while maintaining high beam quality. Watt-range average powers delivered in a diffraction-limited beam will, first of all, increase the standoff-detection distance (*e.g.*, from 10 m to 100 m) for spectroscopic detection of explosives, either liquid (*e.g.*, TATP at 8.6 μm) or solid (*e.g.*, RDX, TNT), as well as for detecting natural-gas leaks (*e.g.*, methane at 7.7 μm). Thus the potential market is sensors for remote detection of explosives and gases such as methane, which at the present time, cannot be remotely sensed due to the lack of high power sources in the 8-10 μm range. The other major potential commercial market is illuminators of thermal imaging platforms in

military applications. Pointing and tracking such platforms from distances of the order of kilometers requires both high average power as well as high beam quality. Furthermore, the proposed phase-locked laser design can be extended the 4-5 μm wavelength range in order to achieve diffraction-limited, usable continuous-wave (CW) powers in excess of 3 W, with at least 15% wallplug efficiency, for applications such as Infrared Countermeasures (IRCM) for both military and civilian applications. The potentially large markets for such high-average-power devices are laser cutting/marking and medical-laser scalpels, thus replacing bulky gas lasers (*e.g.*, CO lasers at 4.6 μm) while providing high average powers at wavelengths not available from gas lasers. Such devices could significantly increase the stand-off distances for detecting toxic gases and explosives in the midwave (MW) IR range, including ammonium-nitrate based explosives.

2. Compact and Ultra-High Resolution Terahertz (THz) Spectroscopic/Fingerprint System. Two Phase I STTR contracts were awarded to Ocis Technology, LLC and NP Photonics, Inc. to develop a compact, tunable, THz-frequency detector that offers ultra-high resolution and room temperature operation over the 1-3 THz range.

While the Far-IR (THz) is nominally defined from ~0.3-10 THz, the frequency range above 1 THz provides a unique spectroscopic probe of the low frequency vibrational modes of materials. Hence, the ability to explore the molecular dynamics of materials in this electromagnetic window will advance our understanding of basic material properties as well as enable new applications, such as the non-destructive detection of complex chemical and biological agents, environmental monitoring, and advanced communications. Such molecule-specific spectroscopy or "fingerprinting" requires spectral resolution at or below ~ 2 MHz, a spectral range that extends to several THz, and frequency tunability. These two Phase I STTR efforts seek to leverage the advantages of low loss nonlinear optical materials and the commercial availability of powerful, compact and tunable lasers to realize significantly enhanced THz difference-frequency generation within guided-wave structures.

The goal of the Ocis Technology effort is to achieve additional enhancements of a THz-frequency source concept that utilizes a novel nested waveguide structure that has been used previously to achieve difference frequency generation (DFG) generation with a power-normalized conversion efficiency of 1.3×10^{-7} W^{-1} (*i.e.*, 23 times larger than the prior state-of-the-art) and a spectral linewidth of 1-2 MHz. The goal of the NP Photonics, Inc. effort is to develop a fiber-based, compact, tunable, THz spectroscopic/fingerprinting system that offers ultra-high resolution (<1 MHz), high sensitivity and room temperature operation over the 1-3 THz range. The THz source is based on a new THz crystal fiber converter combined with high power single-frequency pulsed fiber lasers at eye-safe wavelength ~1550 nm in master oscillator and power amplifier (MOPA) configuration. Detection will be achieved using nonlinear parametric up-conversion that will be coupled into optical fiber and detected using a Geiger-mode avalanche photo-diode (GM-APD). If successful, this technology has the potential for use in point and standoff detection and identification of chemical/biological agents, and has dual use in the detection of concealed weapons.

3. Low Cost Infrared Detector Array for Chemical and Biological Sensing. Two Phase I contracts were awarded to Black Forest Engineering, LLC and New Jersey Microsystems, Inc. to design a MEMS based infrared thermopile detector array that could be used for spectroscopic sensing of chemical and biological agents.

The potential advantages of monolithic thermopile sensor arrays include low cost, very small power consumption, small size, and high sensitivity. The ability to fabricate thermopiles arrays from silicon compatible materials using standard integrated circuit processes holds the potential to improve infrared sensing capabilities within DoD. The thermoelectric coefficients and resistivity of silicon and polycrystalline silicon make them very attractive materials for rugged, inexpensive infrared spectrometers. The New Jersey Microsystems approach concentrates on the MEMS structure and they plan to use crystalline silicon (p and n doped) as the thermoelectric material. The Black Forest Engineering approach will use polycrystalline silicon and silicon carbide on silicon on insulator (SOI) substrates. The research teams will also try to increase absorption with a resonant cavity and absorber layer.

4. Rare-earth doped GaN Lasers on Si. A Phase I STTR contract was awarded to III-N Technology, Inc. to develop electrically-injected lasers on silicon. The objective is to develop new types of optical emitters and amplifiers on silicon that utilize epitaxial growth of III-nitride semiconductors on a Si substrate with in-situ erbium (Er) doping by metalorganic chemical vapor deposition (MOCVD).

The approach is to utilize epitaxial growth of III-nitride semiconductors on Si substrate with in-situ erbium (Er) doping by metalorganic chemical vapor deposition (MOCVD). The approach is based on the successful synthesis of III-nitride UV/visible photonic structures on Si and Er-doped III-nitride photonic structures, achieved jointly by III-N Technology, Inc and Texas Tech University. These photonic structures predominantly exhibit the desired optical emission for optical communication at 1.5 micron. The technical objectives are to (i) further develop MOCVD growth technology for obtaining device quality InGaN on Si, (ii) optimize in-situ Er incorporation into III-nitride device structures, and (iii) develop device fabrication technology for the realization of Er-doped nitride optical amplifiers and emitters active at 1.5 micron. Er-doped III-nitride materials and photonics structures may lead to novel electrically pumped emitters for silicon photonics and optical amplifiers that would possess the advantages of both semiconductor optical amplifiers (small size, electrical pumping, and ability for photonic integration) and Er-doped fiber amplifiers (minimal crosstalk between different wavelength channels in optical networks). The results of the proposed studies will not only yield the science and technology base required for achieving optical emitters and amplifiers on silicon, but will also provide input for the development of suitable quality materials and device designs for a variety of optoelectronic devices active from IR to UV.

5. High-Power Mid-IR Lasers. A Phase II STTR contract was awarded to Pranalytica, Inc. to develop high-performance quantum cascade lasers in the MWIR and LWIR (3-5 and 8-12 microns, respectively). Research progress from the Phase I contract included a successful demonstration of over 1 W room-temperature, continuous wave output from quantum cascade lasers at both 4.0 and 8.0 microns. For this project, DARPA efforts through the Efficient Mid-IR laser program at 4.6 microns were leveraged to increase power at the edge of the MWIR band and into the LWIR for applications, such as, infrared countermeasures and chemical sensing through absorption spectroscopy.

The goal of this Phase II project is to develop two turn-key air-cooled QCL systems in the 3.8-4.2 μm and 8-12 μm spectral regions based on QCLs with 15% WPE and >2 W of optical power. These laser systems will be immediately useful in DIRCM, free space optical communications, and other high power QCL applications. The proposed research is directly responsive to future Army needs in the area of directed infrared countermeasures (DIRCM) and standoff chemical sensing. High performance QCLs will enable new generations of DIRCM systems with higher performance and reliability, lower power consumption with lower cost, thus allowing the protection of many more aircraft. High-power QCLs emitting in the second atmospheric window will find immediate applications in point and remote sensors of chemical warfare agents, explosives, and toxic industrial chemicals, as well as LWIR target illuminators and beacons delivering higher output power with longer run times for a given battery size. Other major application areas that benefit from the commercial availability of high performance MWIR and LWIR QCLs include free-space optical communications, LADAR, DIAL, and noninvasive medical diagnostics.

6. Integration of 360°-Retrodirective Noise Correlating Radar with Panoramic Imager. A Phase II STTR contract was awarded to Physical Domains Inc. to leverage recent breakthroughs in retrodirective noise-correlating (RNC) radar and to develop and demonstrate a new technological capability for imaging sniper bullet trajectories and the local terrain.

Radar-based tracking and imaging tools for the real-time detection and geo-locating of high-velocity threats, such as rocket-propelled grenades and large-caliber bullets, represents a unique and extremely important new technology for Force Protection and Homeland Security. Because the response time for these types of threat scenarios must be tens of milliseconds or less, it is a requirement that the envisioned radar system possesses extremely short detection and acquisition times and should thus be "auto-cued". This system must also provide real-time imaging of the projectile assaults overlaid onto the surrounding 3-D terrain and environment. This Phase II effort will address these requirements by developing the components and algorithms needed for: (i) 360-degree field-of-view retrodirective radar system operation and projectile tracking, (ii) radar hardware-software interface, (iii) radar-camera data fusion, (iv) radar-camera sensor fusion, and (v) field demonstrations of bullet track-track overlay on visible images. This development effort is expected to produce a RNC radar system that is capable of detecting an array of high-velocity threat projectiles and registering their trajectories to a background mapping of the local terrain in real-time to provide visual display tools to warfighters. This technology may ultimately offer a unique capability to the military and law enforcement for countering (and documenting) threats presented by sniper attacks.

7. Minority Carrier Lifetime Measurements in Strained Layer Superlattices (SLS). A Phase II STTR contract was awarded to Power Photonic Inc. to develop a system for measuring the minority carrier lifetime in SLS based on a unique optical modulation technique as well as time resolved photoluminescence.

SLS infrared detectors are significant because they have a theoretical performance limit higher than other infrared detectors, including mercury cadmium telluride detectors. A key metric of infrared detector material is the minority carrier lifetime, which has been difficult to measure in SLS material noting there is much disagreement in the literature. The novelty of Power Photonic's approach stems from the use of the optical modulation response (OMR) measurement, which uses lock-in detection techniques that avoid the instability, noise, and dynamic range issues that arise using other techniques. This will increase the measurement sensitivity up to four orders of magnitude. An added advantage of this OMR technique is the ability to spatially resolve the minority carrier lifetimes across the face of the wafer material as well as completed focal plane arrays. This will reduce manufacturing costs associated with bad materials. Phase I demonstrated the feasibility of the approach and the quality of the measurements that can be made. Phase II will automate the system, improve the system packaging, and improve the measurement speed. This instrument will provide a uniform, repeatable and direct minority carrier lifetime measurement capability that will accelerate progress, improve performance, and reduce costs in SLS detector development.

8. Optically-pumped Gas Fiber Lasers. A Phase II STTR contract was awarded to Precision Photonics to demonstrate an eye-safe optically pumped laser, based on a gas-filled hollow optical fiber, to laze at both near-IR and mid-IR wavelengths.

These lasers will be based on the combination of hollow-fiber and optically pumped-gas technologies. The goal of this project is to demonstrate experimental lasing in the near IR, based on existing models of molecular gases, including acetylene (C_2H_2) and hydrogen cyanide (HCN). Relevant rate constants will be measured in both gases. Both the experimental and theoretical investigations will then be extended to the mid IR. This work will also include the development of the first ion-beam sputtering (IBS) coatings in the mid IR range. Furthermore, optical fibers that guide at both 1.53 micron and 3.0 micron will be developed. Gas lasers can be power scaled and incorporated into fibers reducing their size and allowing for power scaling by cooling the glass surrounding the gas gain media. Also, the pressure of the gas can be changed along with the length of the optical fiber. The mid IR gas-filled hollow optical fiber laser will be able to produce light within the atmospheric transparency window, thus being useful for infrared countermeasures and laser defense. The development of such lasers could be important for IRCM and other mid-wave or near IR sensing and countermeasures.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

No new starts were initiated in FY10.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Energy Guiding and Harvesting through Phonon-Engineered Graphene. A PECASE award was granted to Professor Eric Pop at the University of Illinois, Urbana-Champaign to address current knowledge gaps relating to energy dissipation, transmission and guiding in graphene. This research effort is exploring: (i) the fundamental limitations of ballistic energy transport in graphene through the measurement of electron and photonon transport in ultra-short monolayer and bilayer graphene devices, and (ii) energy guiding in phonon-engineered graphene through the design and measurement of nanostructures with dimensions less than the phonon mean free path length. The proposed research will build a foundation of knowledge for understanding and manipulating energy dissipation and transport in nanoscale electronics. Potential payoffs to the Army include sensor and communication electronics that operate at greater speeds and/or frequencies but that consume less power, hence leading to a reduction in the size and weight of battery power. This work has the potential for discovering new energy-harvesting techniques that would be relevant to all electronic systems used by the Army.

H. Defense University Research Instrumentation Program (DURIP)

As detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Electronics Division managed eight new DURIP projects, totaling $0.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to understand new classes of materials on amorphous substrates, the optical profiling of nanorods, nanowires and nanoparticles, and ferroelectric thin films for use in switchable filter banks for frequency-agile communication systems.

I. DARPA Parametric Optical Processes and Systems (POPS) Program

The goal of the DARPA POPS program is to advance four-wave mixing (FWM) to Si-based photonic structures that will lead to optical processing at data rates beyond 1 Tb/s. ARO is currently managing a project at Cornell University that is focused on using silicon to enhance optical processing. Other projects within this program are focused on using highly non-linear glass optical fibers to achieve the same goals. The high optical confinement of the Si structures enables FWM devices that can operate not only at relatively low powers, but also with short lengths, which will greatly enhance the phase-matching bandwidth. Losses from free carrier absorption (FCA) were mitigated using a reversed-biased diode structure integrated into the FWM waveguide architecture. The DARPA POPS program manager encouraged the ARO Electronics Division to take a lead role in the program by leading multiple teleconferences with the ARL Computational and Information Sciences Directorate (ARL-CISD) to establish an optical networking workshop. This workshop will enable the Army and DoD to gather input and find direction for putting together test-bed architectures proving the advanced capabilities provided by this FWM technology.

J. DARPA Nanoscale Architectures for Coherent Hyper-Optic Sources (NACHOS) Program

The DARPA NACHOS program has been managed for DARPA by ARO since its inception. The program is now completing Phase II. The goal of the program is to demonstrate a sub-wavelength electrically injected semiconductor laser that can be used in next generation photonic networks, such as those used in electronic-photonic integration schemes being pursued at Luxtera. Achievements at the four awardee's labs (the University of Michigan, the University of California - Berkeley, the University of California – San Diego, and the California Institute of Technology) have been made on various approaches throughout the past year. Once significant result from this program has been the recent demonstration of the world's thinnest electrically-injected laser. This laser broke the diffraction limit in the lateral direction by using a metal cladding on an etched nanowire gain medium. Such lasers are currently being pursued in the program to be sub-wavelength in all three dimensions. ARO played a lead role in the program by being the sole government agent on the four awards and co-organizing the 2010 and 2011 IEEE Photonics Society topical meetings which highlight many accomplishements for greater dissemination to the photonics community. This DARPA program pushes the basic research envelope for photonics and advances the frontier in use of plasmonics in lasers to make photonics devices of smaller sizes than ever envisioned.

K. Joint Technology Office (JTO) Multidisciplinary Research Initiative Programs in High Energy Lasers.

ARO currently manages four Multidisciplinary Research Initiative (MRI) programs for JTO on High Energy Lasers that will end in FY11. Along with these four programs, three new MRIs were selected for award through ARO's Electronics Division. The four previous programs focused on fiber laser research, including use of new gain media, new waveguide designs, and passive phase locking models, as well as one program on Gas Lasers. The new MRIs are focused on three different topics: fundamental physics of creating a high power handling optical coating, material loss improvement and beam combining techniques with volume Bragg gratings, and solid core photonic crystal fiber laser development for larger core sizes and suppressed acoustic mode interference. During the past five years, ARO has played a significant role in the four MRIs by organizing a number of workshops, particularly on the fiber laser efforts, to review progress and aid in technology transition and the development of new research programs. NuFern was a key partner on two of the MRIs. As the sole U.S.

producer of custom optical fibers for fiber lasers, their participation was critical and led to two-micron thulium laser products now being used for medical surgery applications.

L. DARPA High Power Efficient and Reliable Lasers (HiPER) Program

The DARPA HiPER Program was funded to understand the thermal management limitations in diode bars toward creating kW level power outputs from single laser bars. Dr. Mike Gerhold of the ARO Electronics Division serves as the DARPA agent for research efforts at the Science Research Laboratory (SRL) which successfully determined how to extract heat from laser bars to such an extent as to make the heterostructure itself the limiting factor in the performance of high power laser bars. An add-on effort based on these results was initiated and SRL will complete four additional tasks in twenty four months. In the First add-on, Task SRL will set-up and test the Micro Cooling Concept impingement cooler to verify its thermal resistance and waste heat removal potential. This task will culminate in the experimental demonstration of waste heat removal of 2.5kW/cm2, thermal resistance of <0.25 K/W and optical power extraction of 170 mW/µm. The second add-on Task will focus on the attachment of 3.6 mm, kW LD bars on an impingement cooler with the goal of demonstrating a high-brightness, kW/bar-cm. The last experimental task will be the design, fabrication and testing of a narrow, 1.8 mm impingement cooler. The main goal of the effort is to extend the methods developed by the PI to laser diode bars capable of kW/Bar-cm output power.

M. DARPA HiPER-II Program

The objective of the DARPA HiPER-II program is to develop compact, efficient and bright laser-diode (LD) sources that will result in extremely light-weight and inexpensive high-energy lasers (HELs) for the U.S. military. The SRL disruptive technologies will increase the power-to-weight ratio of LD pumps for HELs by 20-fold, to 20 W/g from the present state-of-the-art (SOA) of 1W/g. This program follows on the previous DARPA/ARO funded program, HiPER, by taking thermal modeling efforts of HiPER and pushing the pump module forward to create an array of 5 x 5 sq. cm modules in a 10 x 10 array that will be used in the DARPA Adaptive Photonic Phased Locked Elements (APPLE) program together with RIFL (Revolution in Fiber Lasers) to make a steerable HEL weapon with upwards of 300 kW of coherent power in a small package that could fit into a fighter jet or larger plane depending on the form factors. The ARO Electronics Division is providing assistance in leveraging technical knowledge of many related JTO-HEL programs and DARPA's APPLE program to make this a success. ARL-CISD is a co-PI in the new APPLE program, which uses fiber lasers to achieve beam steerable laser arrays.

N. Edgewood Chemical Biological Center (ECBC) Program in Nanoelectronic Architectures for THz-Based Bio-sensing

ARO and ECBC jointly lead and support novel research programs that are advancing the state-of-the-art in nanoelectronic engineering in application areas that have relevance to national defense and security. One fundamental research area that is presently being emphasized by ARO and ECBC is the exploratory investigation of new bio-molecular architectural concepts that can be used to achieve rapid, reagent-less detection and discrimination of biological warfare (BW) agents through the control of multi-photon and multi-wavelength processes at the nanoscale. This program supports multiple ARO single-investigator projects under the support of the Defense Threat Reduction Agency (DTRA) to develop new devices and nanoelectronic architectures that are effective for extracting THz signatures from target bio-molecules. Emphasis will be placed on the new nanosensor concepts and THz/optical measurement methodologies for spectral-based sequencing/identification of genetic molecules.

O. DARPA Efficient Linearized All-Silicon Transmitters ICs (ELASTx) Program

The goal of the ELASTx program is to enable monolithic, ultra high power efficiency, ultra high linearity, millimeter-wave, silicon-based transmitter integrated circuits (ICs) for next-generation military microsystems in areas such as radar and communications. The ARO Electronics Division currently co-manages two university grants within this program that are exploring quasi-optical power combining of Doherty amplifiers, and

asymmetric multilevel outphasing of large numbers of transistor amplifiers. The program will lead to revolutionary increases in power amplification efficiency while simultaneously achieving high linearity for digitally modulated signals.

P. DARPA Thermo-Tunneling Power Generation (TTPG) Program

The goal of the TTPG program is to design and develop radically new thermoelectric architectures that allow for unprecedented high efficiency in converting heat to electricity. The ARO Electronics Division currently co-manages a project within this program that is based on creating vacuum-gaps between spaced thermoelectric materials that allow for effective electron transport and simultaneous thermal isolation. The increased energy conversion efficiency resulting from this program will revolutionize energy extraction from heat and significantly reduce the weight and volume burden of passive devices in all high-power electrical systems.

Q. DARPA High Frequency Integrated Vacuum Electronics (HiFIVE) and THZ Electronics Programs

The long-term vision for the DARPA THZ Electronics program is to develop the critical device and integration technologies necessary to realize compact, high-performance electronic circuits that operate at center frequencies exceeding 10^{12} cycles per second (*i.e.*, 1 THz). The DARPA HiFIVE program will develop a compact, efficient source of electromagnetic energy capable of generating 100 W with 5 GHz bandwidth at 220 GHz using innovative cold cathode and micromachining technologies. The ARO Electronics Division currently co-manages projects within these programs with a goal of using silicon micromachining and MEMS processes to produce precision interaction structures scaled for these extremely small wavelengths. These programs have a high potential impact on military sub-millimeter wave communications, ECM, and radar systems, which is directly responsive to future Army needs in C4ISR and ground mobile wireless communications.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Electronics Division.

A. Absorption and Carrier Transport in P-type Devices

Professor Unil Perera, Georgia State University, Single Investigator Award

The goal of this research effort is to determine the interrelationship of the different hole bands (heavy hole, light hole, and split-off) and how these affect photon absorption and carrier transport in heavily doped p-type detector structures. The detector structures will use III-V material because the split-off band energy in most III-V material is greater than kT at normal temperatures. However, it is still typically only ~10 kT or less so any p-type devices using these materials will have to include the effects of all three hole bands to obtain a full transport model. This is different from many materials (*e.g.*, Si) in which the split-off band energy is only about 0.1 kT at room temperature and can be treated as a single band with one effective mass.

In collaboration with scientists at ARL-SEDD, the investigator successfully developed a full transport model for the split-off response for GaAs/AlGaAs and InGaAsP/AlGaAS based devices, using a Monte Carlo approach that includes the effects of all three hole bands and explains optical properties and carrier transport in III-V structures. This model was verified by growing a GaAs/AlGaAs structure and observing the responsiveness in the 2-4 micron spectral regime. Further studies show the possibility of extending the wavelength range up to 15 microns still operating at or above room temperature. Representative optical transitions and transport pathways that were incorporated in the model are shown in FIGURE 1.

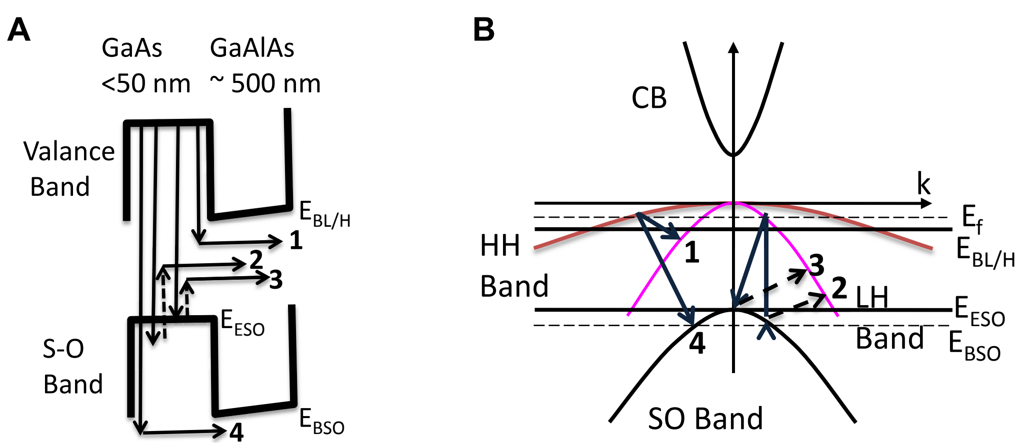

FIGURE 1

Representations of band diagrams of heavily p-type doped III-V barrier devices showing optical transitions. (A) A simplified band diagram illustrates the AlGaAs layer forming barriers to hole transport, while (B) is a more detailed band diagram of GaAs with the barrier levels indicated. E_f is the Fermi level. $E_{BL/H}$ is the barrier for the light hole and heavy hole bands. E_{ESO} is the split-off band maximum in GaAs and E_{BSO} is the AlGaAs split-off band barrier. The arrows show some of the possible optical transitions (pathways) used in the model, as described further in the text.

A transition from the light heavy hole to the light hole band is phonon assisted and the hole has enough energy to surmount the AlGaAs barrier (see FIGURE 1, transition 1). In p-type devices GaAs is heavily doped so the Fermi level is below the valance band maximum. In transition 2, the hole is excited into the split-off band via a direct transition but does not have sufficient energy to surmount the AlGaAs split-off band barrier so it must first decay back to the light hole band before it can be transported across the AlGaAs barrier. Transition 3 is similar to transition 2, but the excitation is phonon assisted. In transition 4, the hole is excited into the split-off band with sufficient energy to surmount the AlGaAs split-off band barrier. Since the position of the Fermi level and the height of the barrier levels depend on the doping, thickness, and aluminum content, these parameters can be adjusted to increase the carrier transport as well as reduce dark current. This model will be used to optimize

design of room temperature infrared detectors. This research could ultimately lead to a mid-wave, uncooled, infrared detector that will yield high resolution and complement existing uncooled, long-wave infrared detectors. The ability to extend to 15 microns also allows for the possibility of an uncooled multi/hyper- spectral detector.

B. Ultra-Fast Magnetoelectronic Devices

Professor Andrew Kent, New York University, Single Investigator Award

This research focuses on the exploration of electron spin-transfer effect for inducing ultra-fast switching responses in nanomagnets. The main goal of this project is to develop a fundamental understanding of coherent control of magnetization dynamics in nanostructures. The investigator has successfully performed experimental studies of electron spin-transfer by passing a current through a "nanopillar" which typically consisted of a thin film stack of magnetic and non-magnetic layers, such as cobalt and copper, respectively (see FIGURE 2). A key aspect of this accomplishment is the ability to grow layers with high control of the anisotrophy of the layer stack sequence so as to achieve magnetization perpendicular to the interface (*i.e.*, results in lower switching currents).

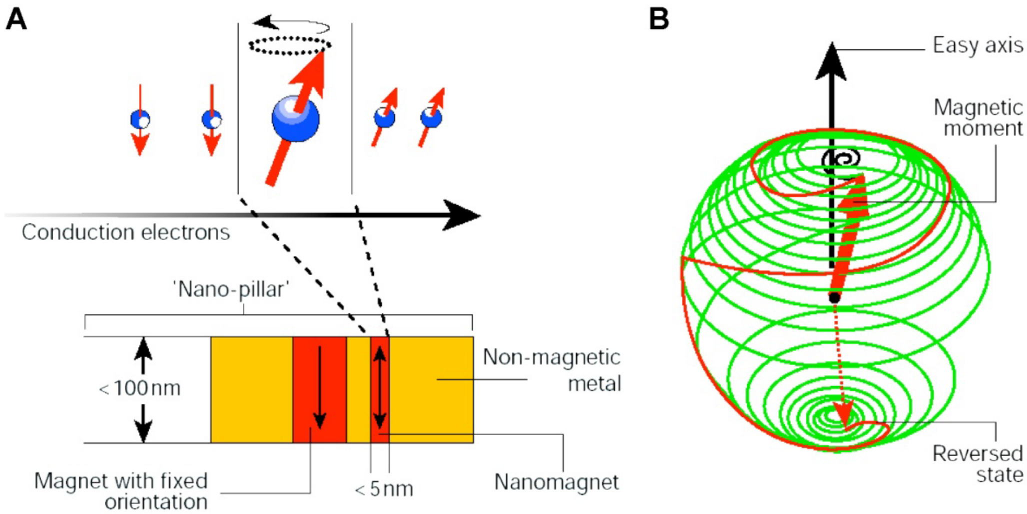

FIGURE 2

Illustration of electron flow through a nanopillar stack and resulting magnetization. (**A**) Alternating magnetic and non-magnetic materials, used to produce electrons with oriented spin-angular momentum. (**B**) Illustration of how the interaction effects of the spin-oriented electrons can influence the magnetization of the thin layer to process and eventually undergo reversal of direction.

A heterogeneous nanomagnet design and the corresponding layer structures that were grown is shown in FIGURE 3. With these innovations in nanopillar design, the research was able to achieve many first-time accomplishments, such as the first demonstration of ultra-fast (<0.3 ns) switching and the first demonstration of ultra-low-energy (<1 pJ) switching.

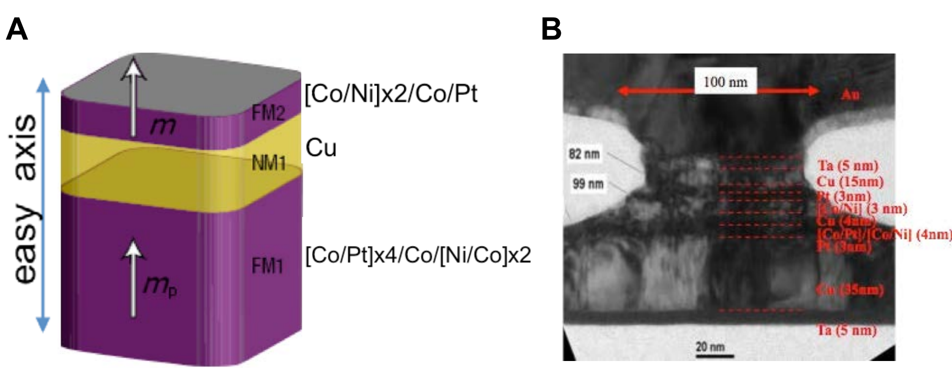

FIGURE 3

Heterogeneous nanomagnet design. (**A**) Nanomagnet design with magnetization perpendicular to layer interfaces. (**B**) Co/Ni-Co/Pt layers grown to produce 100x100 nm^2 and 50x50 nm^2 nanomagnets.

This effort was also the first to perform a comprehensive study of current-pulse induced switching across all switching and current-pulse times. This research is technologically important and lead to a patent being awarded for a new nanomagnet memory concept with the rights being licensed to Spin Transfer Technology, Inc. for commercialization. This may have an impact on a variety of military systems, including threat-agent hyperspectral scanners and detection and ranging radar.

C. Passive Intermodulation Reduction Using External Magnetic Fields

Professor William Chappell, Purdue University, MURI Award

This research focuses on determining the root causes of intermodulation distortion in passive devices and investigating methods to reduce their effects. Professor William Chappell and his research team at Purdue University recently identified a linear-nonlinear interaction that influences the overall nonlinear behavior of many circuits that generate passive intermodulation distortion (PIM). When this interaction is appropriately accounted for, a simple model of the nonlinearity can be used that accurately predicts passive intermodulation distortion levels over wide input power ranges. The nonlinearity in a wireless system can be modeled as a resistor with a cubic (third-order) nonlinear current-voltage curve. It is shown that the apparent multi-ordered nature of most passive nonlinearities can be explained by the interaction between a cubic nonlinear resistor and other linear impedances in the circuit. The behavior of this linear-nonlinear interaction is different for nonlinearities where resistance increases and those where resistance decreases with voltage. Experimental circuits where simulation models account for this linear-nonlinear interaction are used to accurately verify the existence and effects of the interaction by measurement. The interaction is achieved by solving for the voltages and currents of the nonlinear component while accounting for the other (linear) elements in the circuit. Knowledge of this interaction gives a high degree of accuracy when modeling PIM-producing components (*e.g.*, the PIM distortion produced by an SMA connector is accurately predicted by the model both when the connector is included in a through-line topology). This improved model has allowed improved understanding of the physical causes PIM as well as a way to create and improve cancellation and mitigation networks.

The high levels of intermodulation distortion generated by components containing ferromagnetic materials in their conduction paths is likely due to the hysteretic relationship between the magnetization of a ferromagnetic material and any imposed magnetic field. However, it was found that the introduction of an external magnetic field can partially or fully saturate the magnetization of a ferromagnetic metal. This has the effect of decreasing the effective magnetic permeability of the material, lowering the real and imaginary components of impedance. This impedance reduction due to an external magnetic field is known as magneto-impedance (differs from magneto-resistance, a quantum effect), which has been observed for the skin effect and surface impendence in gold-plated SMA connectors where the nickel underplate layer displays magneto-impedance (see FIGURE 4).

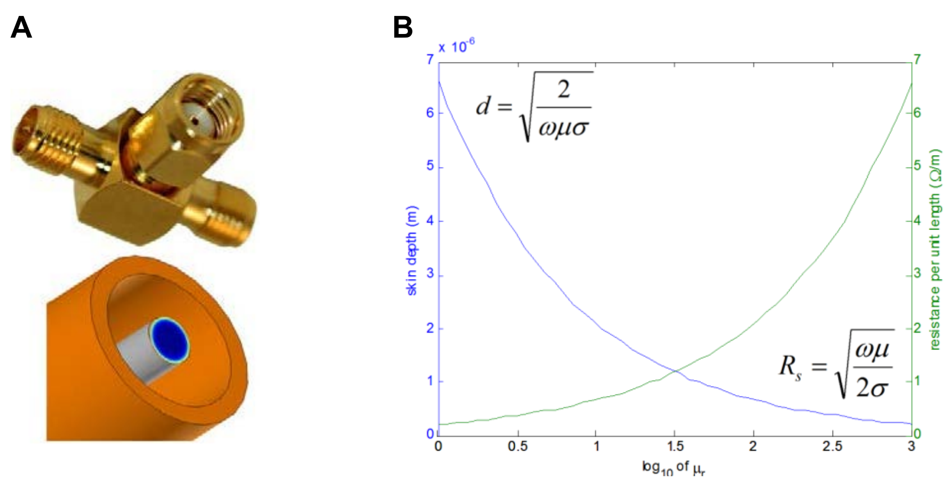

FIGURE 4

Skin effect and surface impedance in a conductor. (**A**) The photo is of a standard SMA connector (top) and a CAD model used in numerical simulations (bottom). The connector body typically is made of brass and plated with gold, using a thin layer of nickel under the gold for adhesion and as a diffusion barrier. (**B**) The non-unity magnetic permeability μ of the nickel layer produces a skin effect in the conductor, which in turn generates a small nonlinear impedance that is the root cause of the passive intermodulation distortion.

A typical hysteresis curve for a magnetic material is shown in Figure 5A. An illustration of the dramatic reduction (up to 40 dB) in PIM under magnetic bias possible with inexpensive RF and microwave connectors is shown in FIGURE 5B. Because of the DC nature of the magnetic source, this type of PIM reduction is broadband in nature, and thus not subject to the bandwidth limitations of many other common cancellation techniques.

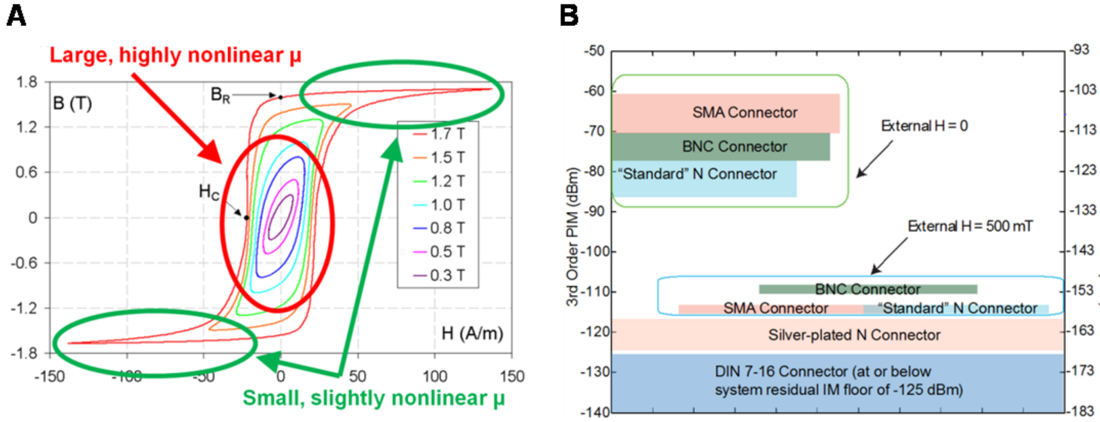

FIGURE 5

PIM reduction using a DC magnetic field. (A) A typical hysteresis curve for a magnetic material. Near the zero field range, the magnetic permeability is large and non-linear, as is evident from the large and rapidly changing slope of the B-H curve. At high magnetic bias, the magnetic permeability is near zero and only slightly nonlinear, resulting in a dramatic reduction in PIM. (B) Illustration of how inexpensive RF and microwave connectors can have a dramatic reduction (up to 40 dB) in PIM under magnetic bias, where they will perform as well as more expensive RF and microwave connectors.

The Purdue research team is working closely with scientists and engineers at the U.S. Army RDECOM Communications-Electronics Research, Development, and Engineering Center, Night Vision and Electronic Sensors Directorate (CERDEC-NVESD), Counter Mine Division in Ft. Belvoir VA, and at the Naval Surface Warfare Center in Crane IN. The PIM mitigation technology will enable very sensitive, high dynamic range detection. The low PIM performance is a key metric for the use of nonlinear detection systems and has the potential to demonstrate powerful next generation tools for the military.

D. Removing Ambiguity in 2D Video Imagery by Use of Context

Professor William Rhodes, Georgia Institute of Technology, MURI Award

The objective of the Human Signatures for Personnel Detection MURI project is to understand the phenomenology underlying the signatures generated by humans, detect those signatures using multiple sensor modalities, and process the signatures in order to detect personnel. As a component of the larger MURI project, this research effort led by Professor Rhodes focused on extracting human signatures from low-resolution video images. The general approach was to exploit knowledge of the 3D background to reduce the uncertainties in the image, thus taking advantage of a greatly increased capability to obtain and manage data on 3D structures. Four stages are involved in the detection process: preprocessing, background modeling, information extraction, and post processing. For this approach, use was made of context based region of importance selection, histogram equalization, background subtraction and morphological filtering techniques. An illustration of this concept with 2D still images is shown with the comparison of a small number of pixels (FIGURE 6A) that were extracted from a 3D scene (FIGURE 6B).

While some information about size in each image could be obtained if the distance to the image was known, it would still be very difficult to detect a motionless human at this resolution. In addition, blurring of background into the image of interest can degrade information exploited with conventional techniques such as shape and color. With motion, the problem can be solved if the scene context is taken into account. If the object was observed in the circled region at the left, it probably represents a moving leaf, a lizard, or some other small animal or insect; if in the circled region on the right, it could represent one or two humans climbing along an ancient pathway. With several frames of video, the probability that the changing pixels represent human(s) can be more accurately determined through the observation of the motion itself.

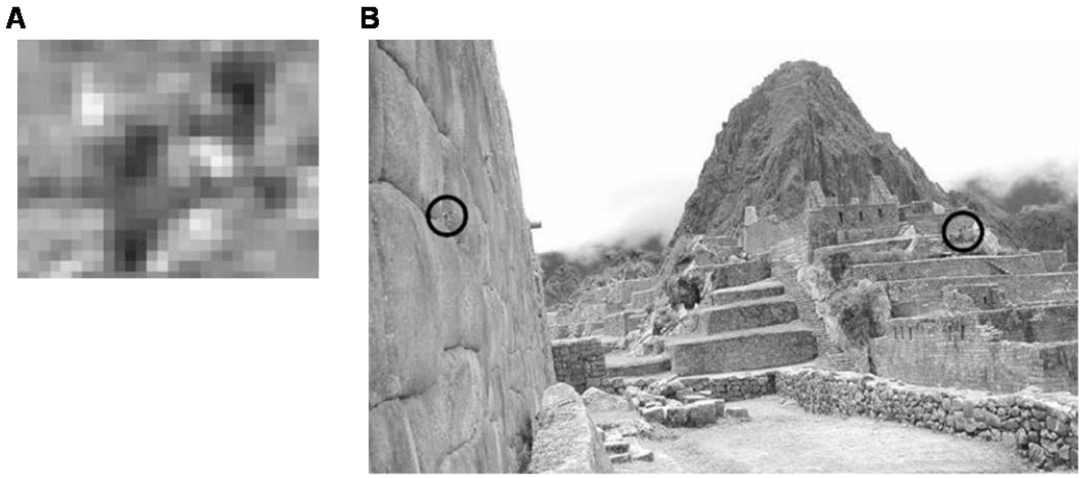

FIGURE 6

2D images extracted from a 3D scene. (A) A small number of pixels, which may or may not correspond to one or more humans, was extracted from (B) a 2D image of a 3D environment. While some information about size in each image could be obtained if the distance to the image was known, it would still be very difficult to detect a motionless human at this resolution. Identifying the location of these pixels within a 3D environment, with two such locations circled in (B), makes determining the likelihood that the pixels represent humans much easier to determine, even in the absence of motion cues.

The investigator successfully developed a system for detection of low resolution objects in video sequences using a single static camera. The system could detect objects as small as 8 pixels in height and 15 pixels in total. It was able to track, handle occlusions, and deal with random noise and other noise due to weather and video conditions. It was further shown that the implementation of histogram equalization improves the contrast between the object and the background but also introduces more noise in the system. In addition, morphological filtering proved to be a valuable method for removing noise that leaked from the background during background subtraction. Future research focuses on the development of algorithms that can operate in real time. This work will lead to an improved capability for automated detection of personnel in scenarios of military interest in regions where the image resolution is low. This research could ultimately addresses a critical DoD need for increased situational awareness and provide a base for higher level information operations, such as classification and behavioral analysis.

E. Nanopatterned Quantum Dot Lasers for High-speed, High-efficiency Operation

Professor Luke Mawst, University of Wisconsin - Madison, Single Investigator Award

Quantum dot (QD) active regions hold potential for realizing extremely high performance semiconductor diode lasers. Unfortunately, these unique features of *ideal* QD active layers have not been fully realized to date. The most successful approach to date of forming QD's is self-assembly under the Stranski-Krastanow (SK) growth mode. However, this approach results in a relatively large distribution of QD sizes leading to significant inhomogeneous broadening of the spectral gain. SK QDs inherently form on top of a two-dimensional "wetting layer", leading to weak electron and hole confinement to the QD, which results in low gain saturation.

Professor Mawst is leading a research effort to investigate the use of dense nanoscale diblock copolymer lithography-based nanofabrication and selective quantum dot growth using metalorganic chemical vapor deposition (MOCVD). These methods will lead to quantum dot active regions in which the injected carriers exhibit *full three-dimensional* nano-scale confinement and elimination of the wetting layer states. The objectives of this project are to (i) develop lasers employing the nano-patterned QD active regions and (ii) investigate the optical gain characteristics of these novel active regions and their potential for increasing the modulation speed of quantum dot lasers.

The investigator recently found that the diblock copolymer nanopatterning process, consisting of a series of pattern-transfers from a dense array of nano-sized holes in a diblock copolymer thin film to a dielectric template mask, allowed for the patterned access to the InP substrate for selective growth of the QDs. SiN_x (10 nm) /

InP(100) substrates were employed using the diblock copolymer process and selective MOCVD growth. High density (~6x10^{10} cm^{-2}) quantum dots were selectively grown (at 610°C) and formed the active region of a laser structure (see FIGURE 7). The TEM image, shown in FIGURE 7B, indicates that the QDs are formed without a wetting layer. This is a significant accomplishment, since such structures will provide full three dimensional carrier confinement, as compared with SK self-assembled QDs. Laser operation (J_{th}~1.1 kA/cm^2 at 20 K) observed from devices with 50-µm-wide stripes and 3.6-mm-long cavities up to temperatures of 170 K as shown in FIGURE 8.

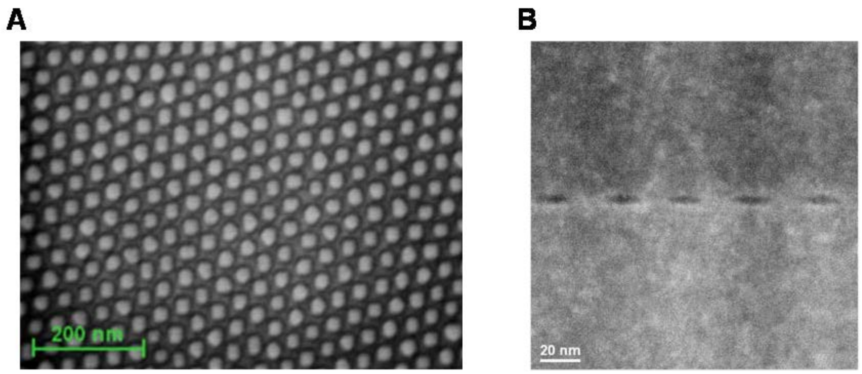

FIGURE 7

Scanning electron micrograph (SEM) and transmission electron micrograph (TEM) of uniform quantum dots. (A) Top-view SEM image of InGaAsP(Q=1.15)/$In_{0.53}Ga_{0.47}As$/InGaAsP(Q=1.15) QDs after selective MOCVD growth; (B) TEM cross-sectional image of the buried QD active region, demonstrating QDs with no wetting layer present.

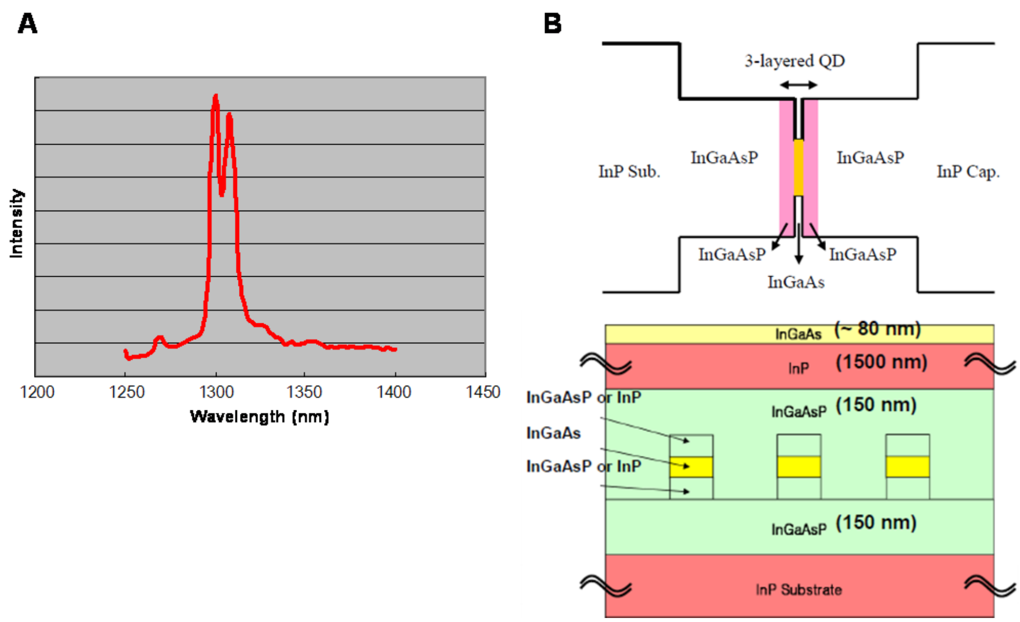

FIGURE 8

Laser oscillation and device structure. (A) The first demonstration of laser oscillation (shown here at 20K) from a nanopatterned QD active region device on an InP substrate; (B) schematic diagram of the nano-patterned active laser structure.

Based on the shorter emission wavelength (~1.3 µm), compared with that of the LT PL spectral peak (~1.4 µm), it appears that lasing may occur on a higher energy (excited state) QD transition. This is an important accomplishment since these data represent the first report of nano-patterned QD active region lasers on an InP substrate. Further improvements in QD growth and pre-etching are expected to lead to ground state emission with lower current densities.

To date, quantum well (QW) active region devices possess the highest overall efficiency and have the highest direct modulation bandwidths of all semiconductor lasers. The use of low-dimensional semiconductor-based, QD-active regions hold potential for realizing even higher power conversion efficiency semiconductor diode lasers, which exhibit ultra high-speed modulation capability, surpassing that of QW based devices. Such compact monolithic sources would allow for ultra-high bandwidth communication and significantly lower input power requirements, which is critical for systems in the field. The realization of these new semiconductor materials with full three dimensional nano-scale carrier confinement, enable basic research studies into the characteristics of optical gain and carrier transport in nanostructures. There is potential to realize significantly higher optical gain at low carrier injection, compared with QW active regions.

F. On-chip Electrical Soliton Oscillators for High-frequency Electronics

Professor Donhee Ham, Harvard University, Single Investigator Award

This research effort focuses on the design and study of electrical soliton oscillators (ESOs) with picosecond (ps) pulse-width capabilities, and on the characterization of their nonlinear signal generation properties. This effort involves the development of concepts that enable the extension of low-microwave one-port ESO prototype designs to high frequencies (*i.e.*, shorter pulses) through the experimental investigation of (i) on-chip ps lumped soliton oscillators (<3 ps pulses), (ii) on-chip ps distributed soliton oscillators (<2 ps pulses), and (iii) on-chip phase-locked soliton oscillators (ps regime).

Solitons are a unique class of pulsed-shaped waves that propagate while maintaining their pulse state (*i.e.*, not breaking into multiple sinusoids) in nonlinear dispersive media, and this research is working towards evolving previous low-microwave linear pulse-shaping concepts of the "circular" and "reflection" type (see FIGURE 9).

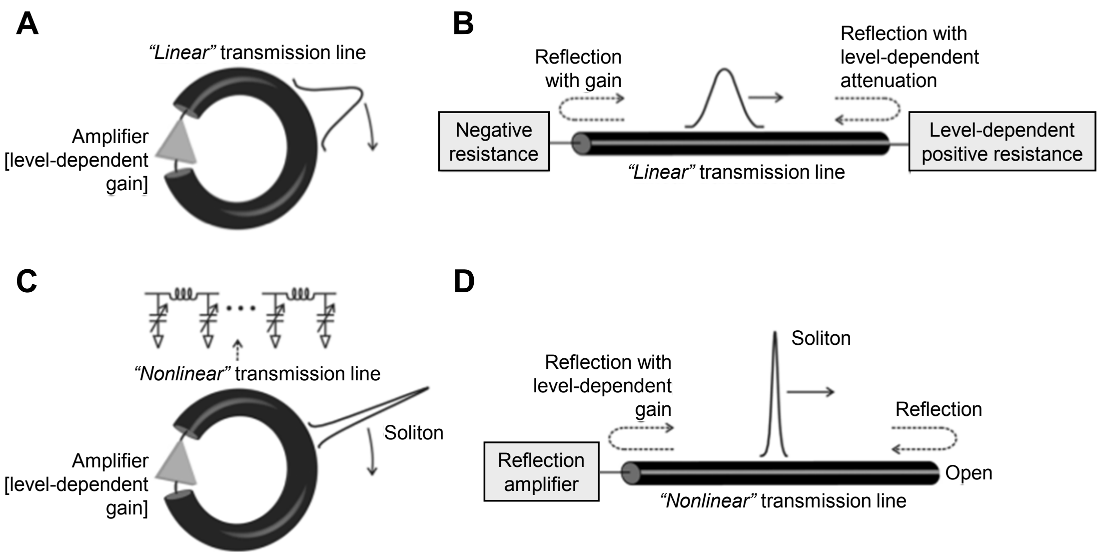

FIGURE 9

Soliton oscillator devices. Four devices are illustrated, including the (A) Cutler concept for a circular linear pulse shaper, (B) Haus variation for a linear reflection-type pulse shaper, (C) Ham concept for a circular soliton oscillator, and (D) Ham concept for a reflection soliton oscillator.

The research team recently achieved several noteworthy accomplishments, including a demonstration of the superiority of the "reflection" soliton oscillator for signal generation over the "circular" concept, which is plagued by chaotic effects. In addition, the team was the first to achieve a phase and mode locked system, which resulted in significant reduction of the phase noise (*i.e.*, ~⁻50 dBc). Also, this effort was the first to carry out experimental investigations into the chaotic processes in circular soliton oscillators. Finally, the team was the first to perform an explicit analysis of phase noise that is globally applicable to all distributed oscillators, including pulsed (*e.g.*, soliton) oscillators. The fundamental amplitude-to-phase noise analysis and the corresponding experimental measurements for validation are shown in FIGURE 10. This work is important

because it is pioneering new areas of high-frequency electrical pulse generation that are relevant to the U.S. Army, such as secure and high-data-rate communications.

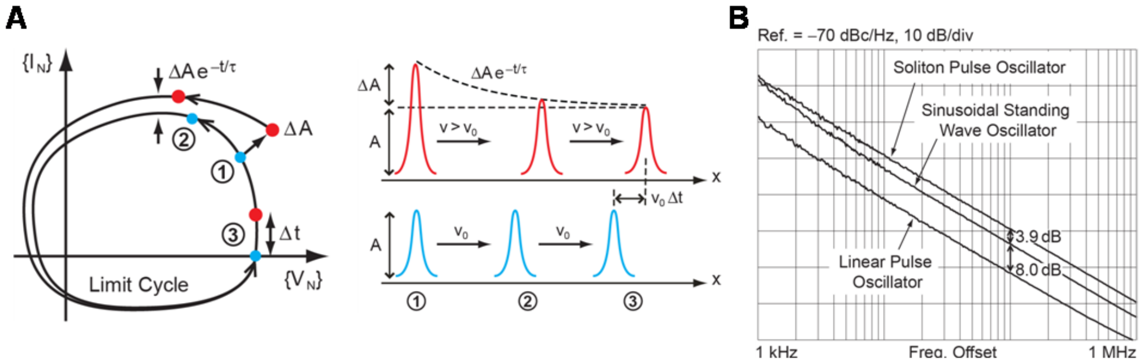

FIGURE 10

Phase noise in soliton oscillator. (A) The limit cycle illustration shows amplitude-to-phase noise conversion in soliton oscillators, and (B) phase noise measurements show the superiority of pulsed oscillators.

G. Incorporating Terrain in Radio Propagation Predictions

Professor G. Brown, Virginia Polytechnic Institute and State University, Single Investigator Award

This goal of this research is to understand how electromagnetic waves scatter from rough dielectric surfaces, incorporating effects as Brewster angle, Norton surface wave, and the effects of surface roughness and loss on wave penetration into the medium. Professor Brown, in close collaboration with ARL-SEDD RF Signal Processing and Modeling Branch, has developed a significantly improved computational model to predict the scattering from a rough 2D dielectric surface, along with its surface wave propagation capabilities. This research is investigating the effects of surface roughness features with wavelengths less than half of the EM wavelength. Validation of the new computational model is being performed using coordinate and wavenumber space methods to provide flat surface checks of the rough surface code, along with analytical approaches to model the scattering from rough surfaces where roughness properties vary along the surface, such as appear over terrain. These surface roughness features are known as large amplitude small period (LASP) roughness features. The impact of LASP on radio wave propagation and scattering is often overlooked by current EM scattering codes. FIGURE 11 shows the magnitude of the surface current produced by a 10-wavelength spatial burst of LASP roughness.

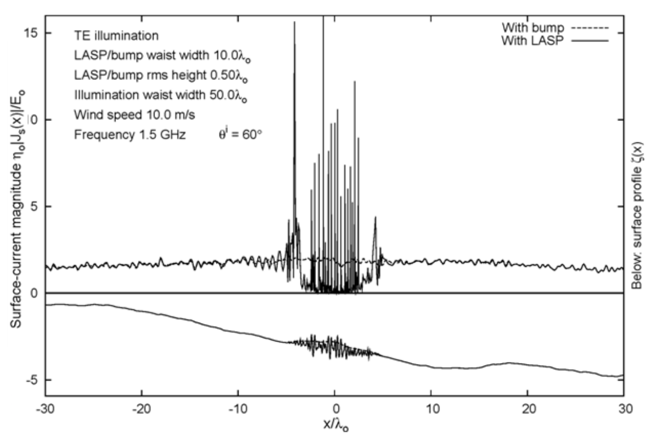

FIGURE 11

Surface current produced by LASP roughness. The magnitude of a surface current produced by a 10-wavelength spatial burst of LASP roughness is superimposed over a lower frequency roughness. The code accurately captures the fine structure of the surface current spikes caused by the LASP features—features that are missed by prior codes that use approximations of the surface topology.

The effects of LASP roughness on terrain backscattering for transverse magnetic (TM) or vertical polarization, and for transverse electric (TE) or horizontal polarization are shown in FIGURE 12. The new code can capture the effect of the LASP features and predicts a stronger normalized radar cross section (NRCS) than previous techniques, leading to more accurate mapping of terrain effects on radio wave propagation. The chief

significance of these results is that they provide the capability to study, in a very accurate and controlled manner, the effects of terrain surface roughness and material on wave propagation and wave scattering for acoustic, radio, and optical frequencies in a unified manner. The primary source of this breakthrough was the prior development of the Method of Ordered Multiple Interactions (MOMI), also supported by ARO under a previous Single Investigator project. These research results were reported at the National Radio Science Meeting in Boulder, CO 6-9 January 2010 and the Joint IEEE Antennas & Propagation and U.S. National Committee of URSI in Toronto, Canada, on July 10-16, 2010. The next step in the research is to compare the propagation results to measurements and investigate the sensitivity of various wave phenomena to surface roughness and material properties, particularly in regard to their effect on radar systems.

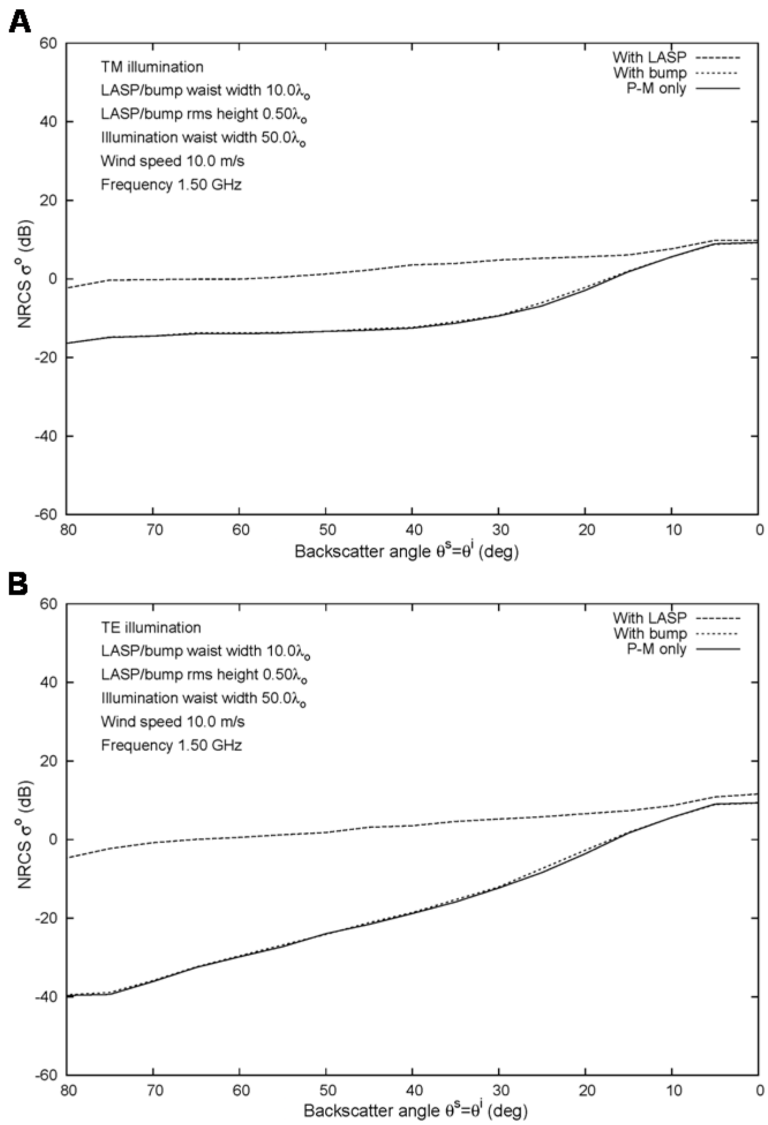

FIGURE 12

Effects of LASP roughness on backscattering. (A) The top graph shows the effect of LASP roughness on the backscattering for transverse magnetic (TM) or vertical polarization. (B) The bottom graph shows the effect of LASP on the backscattering for transverse electric (TE) or horizontal polarization. The new code can capture the effect of the LASP features and predicts a stronger normalized radar cross section than previous techniques, leading to more accurate mapping of terrain effects on radio wave propagation.

If this wave prediction capability is combined with accurate terrain data bases that are just becoming available, it will provide the Soldier with very accurate wave propagation predictions, remote sensing techniques, and remove the uncertainty in radio communications that has previously plagued military forces.

H. Nanofabrication for THz Spectroscopy

Professor Steven Brueck, University of New Mexico, Single Investigator Award

The goal of this research is to explore the nanofabrication of nanofluidic platforms that will enable the control, manipulation and efficient study of bio-molecular transport that can be useful for the optimization of THz spectroscopic sensing. This project is applying hybrid top-down and bottom-up nanofabrication to realize integrated THz and nanofluidic platforms. The specific approach is to combine interferometric lithography with patterned assembly of nanoscale silica particles, resulting in nanochannel arrays as illustrated in FIGURE 13. The project seeks to develop nanochannel platforms with capillary action (*i.e.*, <100 nm) and electrophoresis drive, while maintaining materials and dimensions that are compatible with THz spectroscopic analysis.

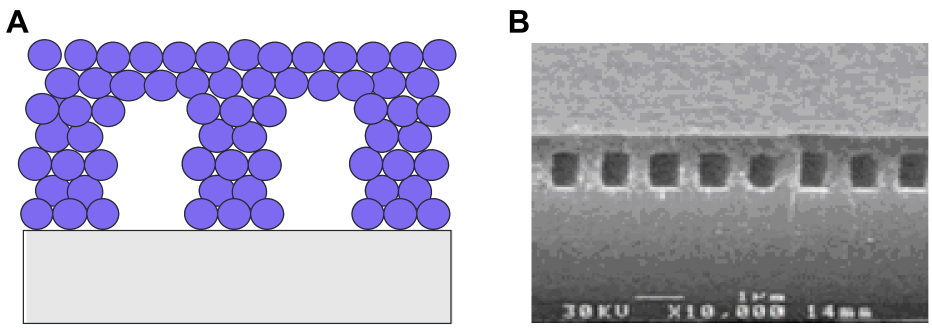

FIGURE 13

Nanochannels. The cartoon in (**A**) illustrates the role of the silica particles in forming the nanochannels, while (**B**) is an actual micrograph of nanochannels.

This research recently led to the synthesis of diffusion-based platforms that were found to enhance signature reproducibility and showed sharp-spectral phenomenology (*i.e.*, linked to elastic modes) for THz spectral measurements on short-chain RNA samples. Studies were also performed on lambda-phage DNA flowing through nanochannel platforms to study the dynamics associated with electrophoresis drive. One result of this new approach is that the movement of DNA within a channel can be tracked as a function of position via the application of negative (and positive) voltage along the nanochannel (see FIGURE 14).

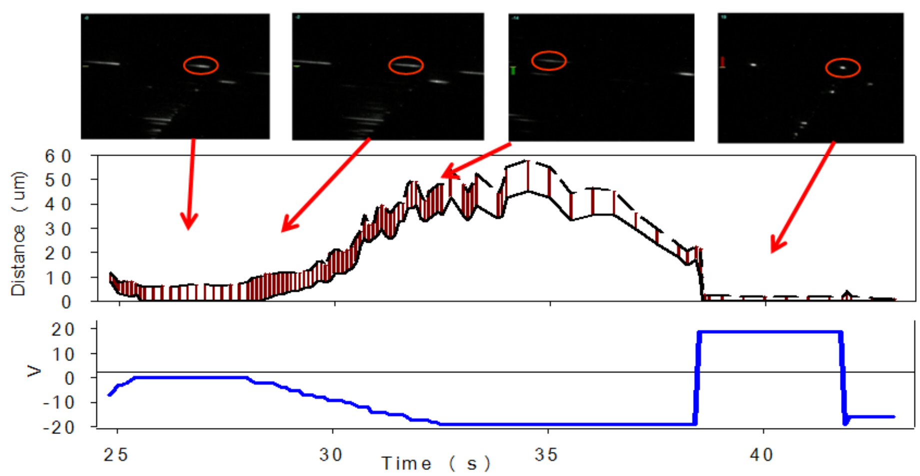

FIGURE 14

Diffusion-based platform measurement examples. (Top) Time snap-shot images of fluorescently labeled DNA chains contained inside a nanochannel array with one DNA chain designated by a red circle. (Middle) The position of the DNA (i.e., inside the red circle) is graphed as a function of time. The arrows indicate position at the time of the snap-shot images (Bottom) and the voltage (V) that was applied as a function of time.

This research effort and its recent accomplishment are important for establishing the scientific methodologies required for precise control of DNA flow within nanochannels. This work will be important for realizing

extremely stable flow and very reproducible THz spectral signatures, which are needed for defining new detection and identification methodologies of biological threat agents.

I. Continuously Spatial-wavelength-tunable Nanowire Lasers On a Single Chip

Professor Cun-Zheng Ning, Arizona State University, Single Investigator Award

This project is pursuing several goals, including (i) to develop a strategy and methods for systematically and controllably growing semiconductor alloy nanowires with variable or continuous spatial composition grading on a single substrate, and (ii) to demonstrate multi-wavelength (or spatially tunable) lasing from such nanowire wafers. These objectives are being pursued through a systematic investigation involving the parametric-dependent study of the chemical vapor deposition of nanowires and other materials and their optical characterization. The experimental approach also involves fabrication of vertical array of nanowires for device fabrication.

This research has led to several important accomplishments in FY10. First, the researcher demonstrated lasing under optical pumping in the wavelength range 500-700 nm (at 77 K) and 550-650 nm at room temperature (see FIGURE 15). This is the widest tuning range on a single substrate of any semiconductor based laser source.

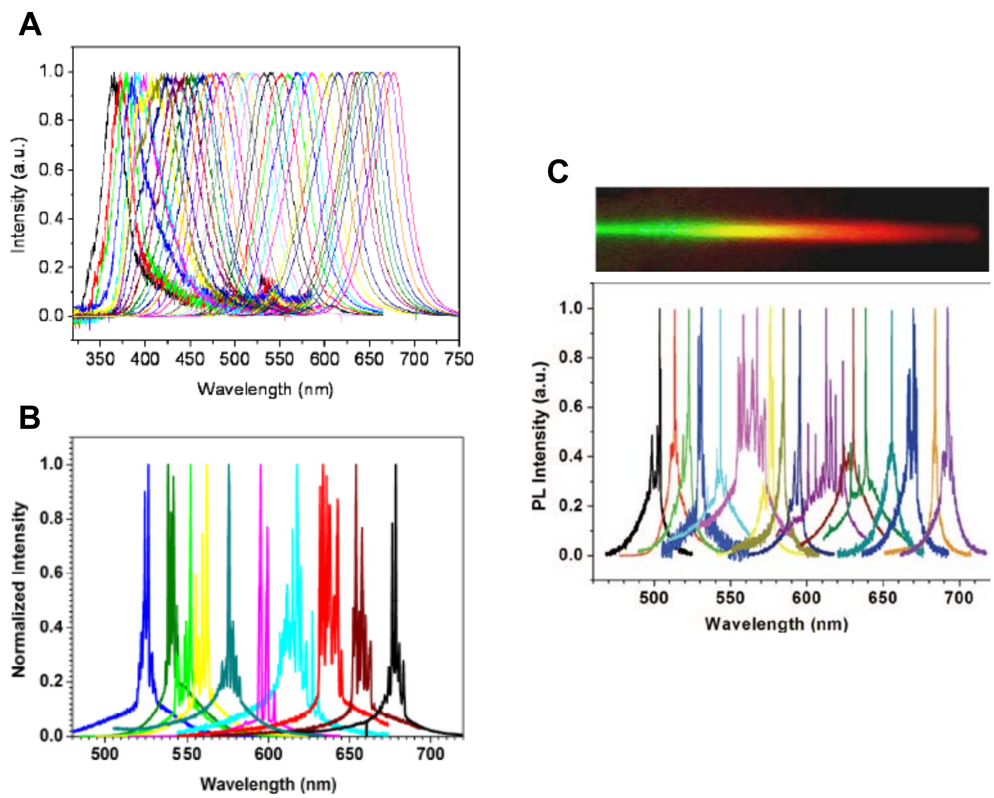

FIGURE 15

Optical pumped lasing on single substrate. Lasing on a single substrate is shown from (A) 500-700 nm at 77K and (B) 550-650 nm at room temperature. (C) The top portion of this figure displays photoluminescence over the entire visible spectrum of a 1.2-cm long nanowire sample, showing bandgap changes from left to right, while the bottom displays a spatial-resolved microscope photoluminescence collected at points along the substrates. The sharp spectral lines indicate lasing action occurring at high optical pumping.

Second, the investigator identified quaternary alloy nanomaterials ZnCdSSe in the entire bandgap range between that of ZnS (350 nm) and CdSe (700 nm). Quaternary alloy nanomaterials have never before been demonstrated in any nanomaterials form including nanowires or nanoparticles. In addition, ZnCdSSe materials have never before been grown in the complete bandgap range. They achieved the light emission in the complete visible spectrum on a single substrate for the first time

Third, the investigator and his team successfully demonstrated a vertical array of high quality CdSe nanowires grown from AAO pore templates (see Figure 16). The growth of such vertical array growth without requiring single crystal substrate (and thus not limited by lattice matching requirement) will benefit many applications, especially electrical injection devices such as lasers and detectors.

Forth, the researchers demonstrated the growth of high quality PbS nanowires with strong PL in mid-infrared wavelength range. Alloying between PbS and ZnCdS can provide potentially a material capability from mid-infrared all the way to UV on a single substrate.

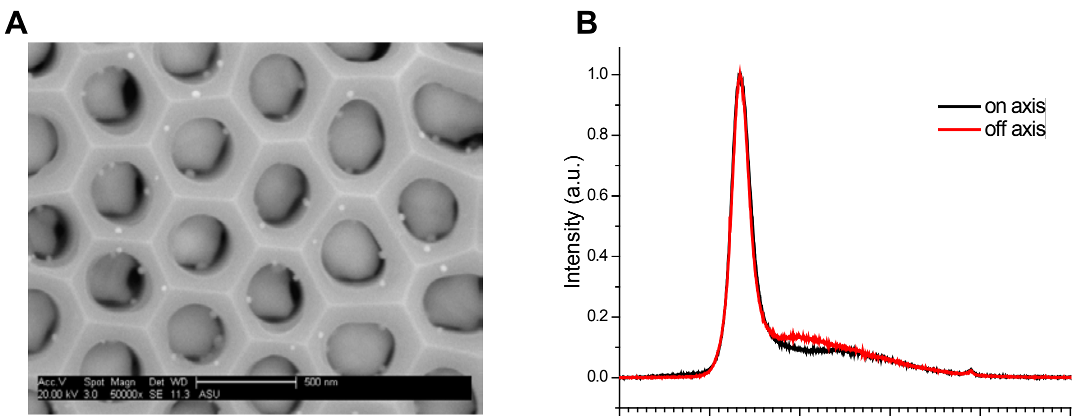

FIGURE 16

Nanowires grown in AAO. (**A**) A micrograph of a top view of the nanowires shows a pore diameter of ~200 nm. (**B**) The corresponding photoluminescence spectra show almost identical linewidth for the wires grown in the pores and for the growth without pore templates.

Collectively, these materials capabilities will have potential application in many areas of interest to the Army. Producing semiconductor materials with a wide range of bandgaps from UV to red and mid-infrared on a single substrate will allow multispectral infrared detection camera with multiple wavelengths, or even spectrometer on-a-chip in the mid-infrared wavelength range. The unprecedented wavelength range of light emission on a single substrate could be used for high efficiency flexible displays, a capability that is currently being pursued by the Army using organic materials. The inorganic materials being characterized by this research effort may be advantageous due to longer luminescence lifetimes and material stability. Finally, widely tunable lasing on a single substrate can potentially be used for multi-agent detection or sensing on a compact platform.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Formation of Defect Structures and Electrical Transport in VO_X

Investigator: Zhi-Gang Yu, SRI International, Single Investigator Award
Recipients: CERDEC-NVESD; L3 Communications (L3-Com)

The goal of this basic research effort was to achieve a comprehensive understanding of the electronic and lattice structures in highly disordered vanadium oxide (VOx), in particular those associated with defect microstructures, and their impact on the temperature- and time-dependent electrical transport in VOx. In the course of this theoretical effort, the investigator developed physical pictures and modeling tools to describe defect structures, electrical transport, and optical properties in VOx systems. An important discovery was that the total conductivity in VOx was not the summation of two channels, as in amorphous silicon, but rather that it switches from variable range hopping at low temperatures to nearest neighbor hopping at room temperature. This knowledge led to a calculation of the 1/f noise in this material.

This theoretical understanding of defect structures, electrical transport, and optical properties in VOx has been transitioned to CERDEC-NVESD and L3-Com, and is being used by these groups to identify VOx and other materials with appropriate compositions and defect structures for improved detector materials. This research has the potential to increase the performance of uncooled infrared detectors such that that low-cost imagers can take over some of the current applications of higher cost, cooled, imagers.

B. Polysilicon Electrode Device

Investigator: James Tour, Rice University, Single Investigator Award
Recipient: Privatran Corp.

Professor James Tour's research group has fabricated new Poly-Si/SiO_x/Poly-Si devices with 10 nm SiO_x thickness. These polysilicon devices allow for multistate switching at moderate writing/erasing voltages (~5-7 volts) and pulsewidths (~30 ms), as shown in FIGURE 17. Professor Tour's group is also utilizing multi-walled CNT electrodes to localize the Polysilicon devices to precisely defined positions. Here, high current flowing through a CNT is used to create a nanogap region that allows for atomic-scale positioning of the device to be characterized. These evolving technological capabilities are significant because they represent a new class of ultra-small voltage-switched memory devices that can be used to realize ultra-dense memory arrays.

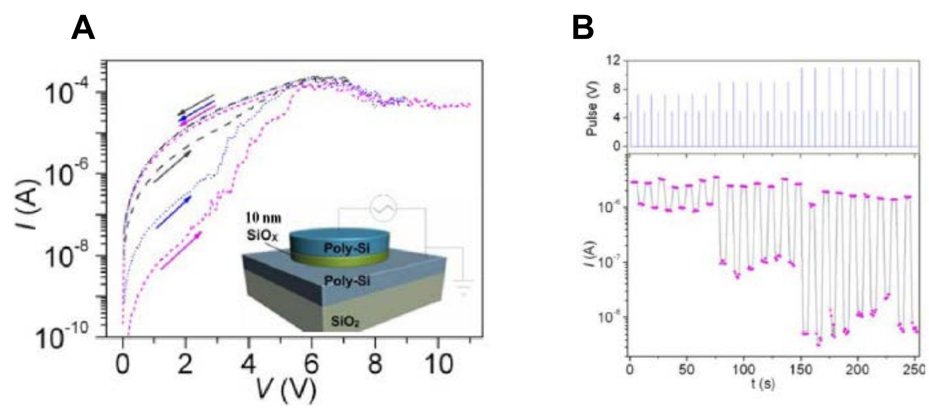

FIGURE 17

Polysilicon electrode device. (A) The graph shows the IV curves and a schematic of device, while (B) the graphs are a demonstration of multiple resistance states measured at 1 V (lower) with the application of different write voltages (5 V) and erase voltages (7 V, 9 V, and 11 V), as indicated (upper).

Professor Tour is presently working with Privatran Corp. to develop 1K memory arrays for demonstration under a Phase II STTR project. This work offers the potential for the significantly up-scaling of high-speed memory technology which will be required for capturing, storing and processing the massive amount of data that is associated with integrated sensor systems of relevance to military applications.

C. Phenomenology of the Interaction between Electromagnetic Fields and Electronic Devices
Investigator: Michael Steer, North Carolina State University (NCSU), MURI Award
Recipients: ARL-SEDD; JIEDDO

The goal of this research project is to study of the interaction between electromagnetic fields and electronic devices. During the course of the program, the investigators discovered a new phenomenology that offers the capability to predict re-radiated signals that can occur when an electronic device is illuminated with an electromagnetic waveform. This phenomenology formed the theoretical basis and rationale for a collaborative effort between ARL-SEDD, NCSU, a North Carolina small business, and a defense contractor supported by the Joint IED Defeat Organization (JIEDDO). The research results will improve the performance of electronic warfare systems.

D. Alignment Tolerant Optical Interconnects for Radar Remoting
Investigator: Anis Husain, Ziva Corp, SBIR Contract
Recipients: Lockheed Martin; Army Program Executive Office (PEO) for Missiles & Space

During Phase II of the SBIR effort, Ziva Corp. advanced its optical interconnect approach up to TRL 5, which involved the fabrication of an interconnect prototype with four coarse wavelength division multiplexing (CWDM) channels. Ziva demonstrated errorless data transmission (Bit Error Rate or BER) of $<10^{-12}$ at 2.5 Gbps over 1 km distance with a 1.2 GHz bandwidth reflective semiconductor optical amplifier (RSOA).

Lockheed Martin confirmed that the Ziva Corp. transmit receive system successfully passed BER of 10^{-12} at GigE (Giga-Ethernet) speed over a temperature range from -31.5 °C up to +73 °C. This accomplishment showed promise for insertion into the Army's Medium Extended Air Defense System (MEADS) radar system. Lockheed Martin is the lead on this effort for the MEADS development, which is run by the Army's PEO Missiles & Space organization. This technology transition will be made to use Ziva's interconnect approach for use on the radar antenna and in moving the antenna away from its CPU (remoting), as shown in FIGURE 18. Lockheed Martin has invested its own resources in the Phase II enhancement project to guide the transition.

Optical interconnects used in radar remoting must pass through a fully rotatable slip-ring to a CPU up to a kilometer away. A CWDM approach (with multiple channels per fiber) reduces the number of optical fibers needed to connect to the antenna array's many transceivers to the network, and thus meeting the limit on the number of fibers that can connect through the slip-ring. More common vertical cavity surface emitting laser (VCSEL) approaches require one laser per fiber, and would not meet this limit. Ziva is using Superluminescent LEDs (or SLEDs) as continuous wave light sources at the CPU location, and RSOAs are used at the radar antenna. This unique optical interconnect approach will provide a highly robust, high speed, scalable and reliable optical interconnect solution to the problem of interconnecting sensors/radar etc., to remote multiple processors on a board. The optical extender solution is robust and reliable because it is not based on non-resonant devices (no lasers), but on SLEDs. The ruggedness of SLEDs indicates superior reliability compared to conventional VCSELs. Ziva's concept is also capable of very high speed data transfer enabled by utilizing a pre-emphasis driver for the RSOA and scalable in data rate via CWDM from Gbps to 40 Gbps. Later this year the per channel data rate will be increased from 2.5 Gbps to 10 Gbps noting that extension to 40 Gbps is possible in using compact and robust format.

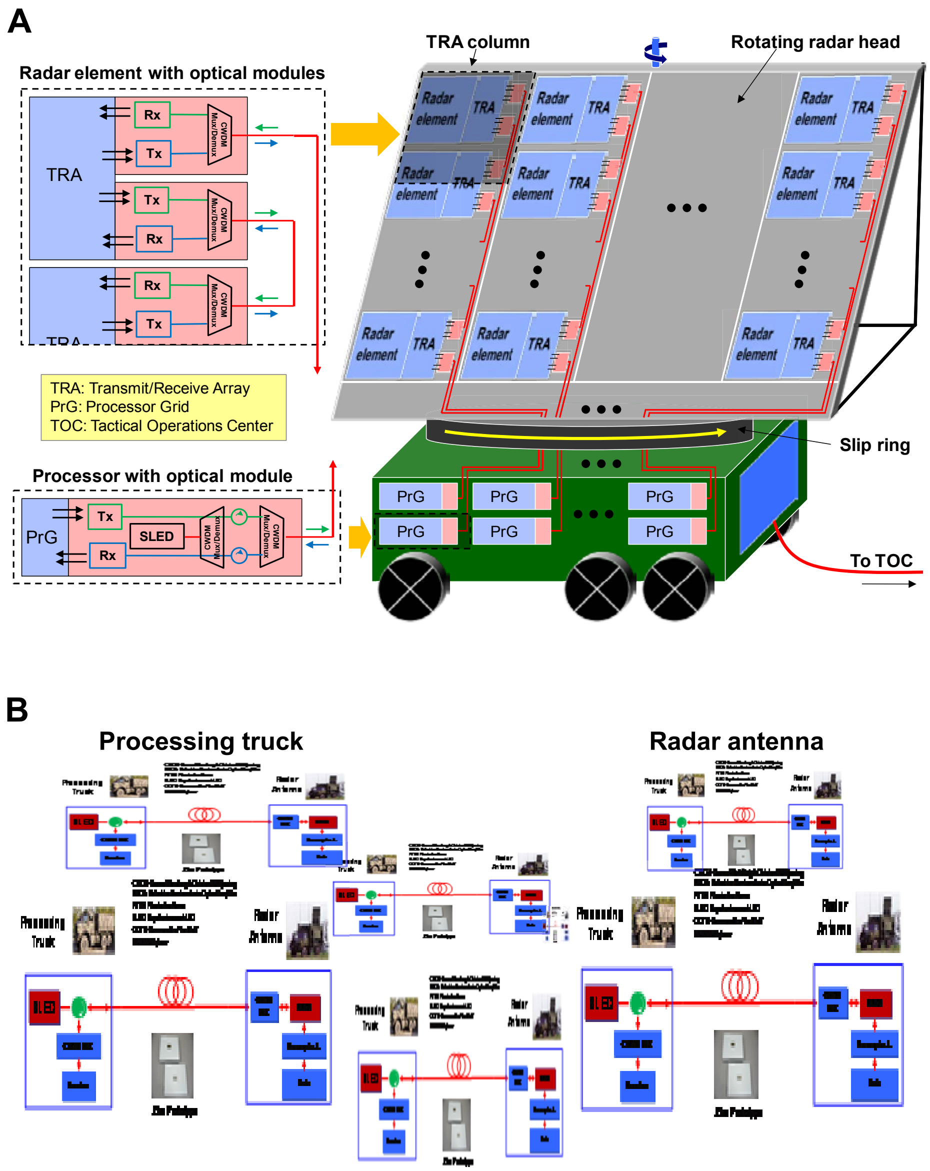

FIGURE 18

Two applications of Ziva OI links. Applications of Ziva OI links include (**A**) radar remoting and (**B**) high-speed data distribution on the radar phased array.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Scale Effect in Flexoelectricity

Professor Xiaoning Jiang, NCSU

Recent research progress on flexoelectricity has suggested that dramatic enhancement of effective piezoelectric properties is attainable through flexoelectric (FE) scale effects. Flexoelectricity is created when *non-uniform* strain/stress locally changes the piezoelectric tensor. This can occur even in centrosymmetric crystals when the strain/stress gradient breaks the inversion symmetry. Initial predictions for 50 nanometer size objects of barium strontium titanate (BST) show increases in the effective d33 piezoelectric coefficient by a factor of 1,000 over the bulk, which is higher than any known d33. However, these FE structures are not currently realizable due to inherent nanofabrication challenges and the fundamental challenges in charge separations.

In FY11, the PI plans to fabricate microbeams and pyramids at micron sizes (see FIGURE 19A) and then evaluate the scaling effect. The investigator will use a charge measurement system based on a modified Sawyer-Tower circuit to measure the effective d33 (see FIGURE 19B).

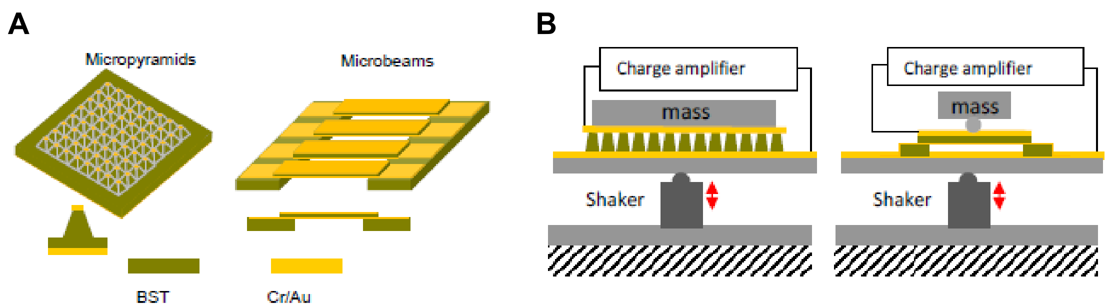

FIGURE 19

Flexoelectricity experimentation. The investigator will (**A**) fabricate proposed flexoelectric structures and will (**B**) use a charge measurement system based on a modified Sawyer-Tower circuit.

FE micro/nanostructrues will enable the development of novel seismic sensors, acoustic sensors, electromagnetic sensors and uncooled infrared detectors. If the high expected values are obtained they will also enable more efficient energy harvesting from ambient environment (thermal, vibration, EM waves, etc.) for self-powered wireless sensors for multimodal sensing. Lastly, the high electrical energy density will enable actuators with low driving voltages and power consumption, which could result in new miniaturized robots for use by the Army.

B. Electronic Properties of Graphene Using Scanning Probe Microscopy

Professor Brian LeRoy, University of Arizona

The novel linear dispersion relation of graphene gives rise to Dirac fermions, which are likely to lead to entirely new types of devices, from transistors to sensors. However, before these devices can be realized, the fundamental limits of graphene performance must be understood as well as finding ways to control the electronic bandstructure. To accomplish these goals, novel probes and characterization methodologies are necessary (see FIGURE 20).

It is anticipated that by using scanning probe microscopy, this project will successfully probe the electronic behavior on the nanometer length scale, which will enable fundamental investigations on important questions such as, what factors limit mobility in graphene devices. In FY11, this project will explore the effect of doping on mobility and determine the origin of electron and hole puddles in the local density of states. Furthermore,

scanning probe microscopy will be used to probe the effect of the graphene-substrate interaction on the electronic bandstructure. Control of the bandgap in graphene can be accomplished by changing its width with selective voltage pulses from the microscope tip. Understanding and controlling all of these phenomena is critical in order to create new types of device; therefore, this work has the potential for making discoveries that will lead to the next generation of ultra-fast and/or ultra-high-frequency electronic devices.

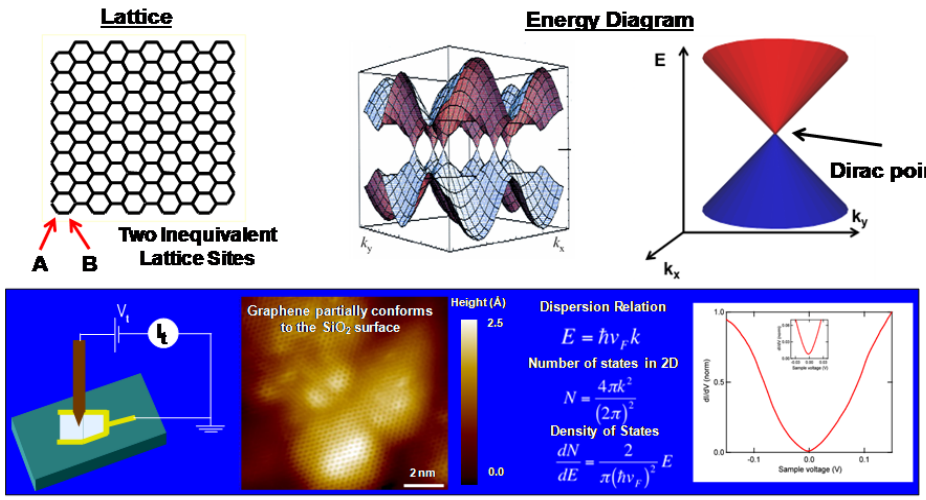

FIGURE 20

Graphene Dirac points. (Upper) Monolayer graphene geometry and bandstructure characteristics illustrate the source and location of Dirac points and (lower) a probe-based characterization methodology that affords one the ability to map the Dirac points.

C. Investigation of Dual-Mode, Electron/Ion Vacuum Microelectric Devices

Professor Brian Stoner, RTI International, Inc.

Vacuum electronic devices operate by controlling the interaction between electromagnetic fields and electrons moving in a vacuum. Thus, they are single-carrier devices. Solid-state semiconductor devices, on the other hand, can use both electrons and holes (electron vacancies) to move charge, enabling the complementary device structures that are the basis of CMOS technology. If the same capability were available in vacuum electronic technology, it could lead to an entirely new class of devices that would merge the advanced circuit capabilities available from CMOS technology with the high carrier mobility and high-temperature, radiation-resistant performance available from vacuum electronics. Professor Stoner's group has developed a new concept for a dual-mode vacuum microelectronic device (D-VMD) and is working to advance the fundamental understanding of the role of ions as charge carriers. In FY11 the team will use computational modeling of candidate device topologies for controlling electron and ion flow, investigate selected single or combinations of multiple background gases to optimize ion generation, and assess ion mobility and its affect on high-frequency operation to prove the concept. An SEM of a five-panel micro-ionization source, fabricated using MEMS technology, reveals that it is possible to fabricate vacuum microelectronic devices (see FIGURE 21).

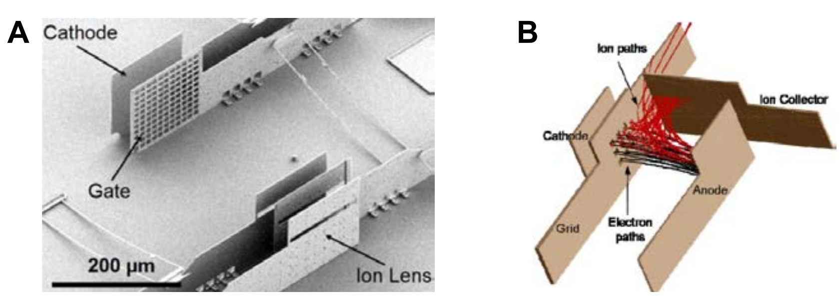

FIGURE 21

Five-panel micro-ionization source. (A) An SEM of a five-panel micro-ionization source, fabricated using MEMS technology, reveals the feasibility of constructing vacuum microelectronic devices, and (B) a schematic generated from a computational model of electron (black) and ion (red/gray) trajectories in the proposed D-VMD.

While the fundamental operation is significantly different, the proposed device is hypothesized to behave like a conventional CMOS inverter. The efficiency of charge modulation is expected to be a function of many variables, including: electrode geometry, electric field strength, frequency of operation, ion mass/mobility, and others. This proposed research is designed to study these factors with an interest in both understanding the phenomena as well as improving next generation device designs. If successful, the D-VMD will generate a number of new capabilities, such as sensing and communication in harsh environments.

D. Investigating Array Size Scalability and Longitudinal Mode Control for Laser Beam Combining

Professor Lin Zhu, Clemson University

The goal of this STIR project is to investigate the scalability limits of a unique approach to scale power from a semiconductor laser. The design of the laser is done through careful placement of diffraction gratings that act both to expand the mode volume and to create a folded supercavity along the length of the gain chip. Where semiconductor laser bars normally have lateral placement of individual arrays, angled etching of diffraction gratings provides a means to make a single folded supercavity where the entire bar is made into a laser with coherent emission. Previous efforts, such as SCOWL or IAG (Index Ant-guiding), provide alternate approaches but they both couple separate lasers to a common emitted mode. The folded approach goes one step further in combining each edge-emitter with the next into a common supercavity. While experimental efforts were supported under a DARPA Young Faculty Award, the theoretical aspects are being explored under this STIR. The important question for high energy laser (directed energy) experts is to find the scalability limits to make over a kilowatt from a single bar with coherent single mode emission, i.e. with longitudinal mode control. With the recent demonstration of over a kW of laser power from a single laser bar, the coherent combining and mode control of such emission is an important next step to making miniature weapons and sources for cutting, welding, and directed energy applications. It is anticipated that this STIR project will generate data that addresses the theoretical nature of this question. Based on the information provided through this award, larger experimental studies may be added.

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CHAPTER 6: ENVIRONMENTAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Environmental Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Environmental Sciences Division supports basic research to advance the Army and Nation's knowledge and understanding of the atmosphere, the terrestrial domain of the natural environment, and habitation therein by the Soldier. Specifically, the goals of the Division are to develop first-principle knowledge of the physical, chemical, and biological basis of atmospheric and terrestrial processes at Army relevant spatial and temporal scales, as well as improve fundamental understanding of lower atmosphere, air-land interface, and near-surface environment, and their dynamic behavior and complexity at those scales. The research results stimulate future studies and seek to maintain U.S. dominance at the forefront of research in military-relevant areas of the environmental sciences.

2. Potential Applications. The research efforts managed by the Environmental Sciences Division provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO in the environmental sciences will impact and leverage environmental factors in favor of the Army to take advantage of environmental weakness of adversary systems, optimize the design of new systems, and ensure mission sustainability. The capability to understand at a fundamental level the atmosphere and remotely sense and interpret Earth's surface feature (both natural and anthropogenic) are critical for mission success.

3. Coordination with Other Divisions and Agencies. Because the natural environment is, by nature, a highly complex and dynamic system characterized by complicated feedbacks, multidisciplinary approaches are fundamental to environmental science and are addressed in every aspect of this Division's basic research program. For this reason, the Environmental Sciences Division's basic research program is developed in conjunction with the ARL Battlespace Environments Division and the laboratories of the U.S. Army Corps of Engineers (USACE), the Army Communications-Electronics Research, Development, and Engineering Center, Night Vision and Electronic Sensors Directorate (CERDEC-NVESD) Countermine Division, and the Army Engineer School. The program is also coordinated with related programs in other Department of Defense agencies including the Department of Navy, the US Marine Corps, the Department of the Air Force, the Defense Advanced Research Projects Agency (DARPA), the Strategic Environmental Research and Development Program (SERDP), and the Environmental Security Technology Certification Program (ESTCP). Across the U.S. Government, coordination with the U.S. Environmental Protection Agency (EPA), National Aeronautics and Space Administration (NASA), National Oceanic and Atmospheric Administration (NOAA), National Science Foundation (NSF), and US DOA Agricultural Research Service occur as a matter of standard operations.

B. Program Areas

To meet the long-term program goals described in the previous section, the Environmental Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the

evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these three Program Areas: (i) Atmospheric Science, (ii) Terrestrial Sciences, and (iii) Habitation Science. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Atmospheric Science. The objective of this Program Area is to explore and understand the behavior and effects of the atmospheric boundary layer over land. This understanding is mission critical since intelligence planning for the battlefield depends on a full and timely knowledge of atmospheric conditions and their effects on operations, weapon systems, and the Soldier. Knowledge of the atmosphere and its effects on Soldiers and sensor systems are essential for command and control as well as visualization of the battlefield at all echelons. The ultimate goal of this Program Area is to uncover methods and tools for the Army to address the wide spectrum of conditions and influences of the atmospheric boundary layer on Army operations and systems.

2. Terrestrial Sciences. The goal of this Program Area is to improve the fundamental understanding of terrain and land-based phenomena. By investigating the broad spectrum of terrain and land-based phenomena that affect the Army, the long-term applications of discoveries made through this program will significantly enhance the Army's ability to fully achieve its Future Force vision for full-spectrum operations. The achievement of this vision will require a sustained investment in Terrestrial Sciences basic research that addresses the scientific challenges identified as capability gaps for the Army's Future Force, together with those issues understood to be critical to the stewardship of Army installations necessary to insure the sustainability of Army training and testing lands and the remediation of Army contaminated sites. Because the natural environment is, by nature, a highly complex and dynamic system characterized by complicated feedbacks, there is an increasing need for multidisciplinary approaches to address the multifaceted problems that are addressed by the ARO Terrestrial Sciences basic research program. This extramural research program is developed in conjunction with the laboratories of the USACE Engineer Research and Development Center (ERDC), the Countermine Division of CERDEC-NVESD, and the Army Engineer School, with input from land managers at several Army installations.

3. Habitation Science. The goal of this Program Area is to explore engineered biological processes, membrane processes for water purification, energy recovery and conversion, and resource reuse and transformation. Research efforts within this program are exploring radically new unit operations with the potential to maximize recovery of usable energy via physical, chemical and biological processes. Such operations need to simultaneously minimize system mass, volume and power while controlling the amount, composition and release of reaction by-products. This Program Area also coordinates efforts, and leverages funding with other agencies, including Product Manager Force Sustainment Systems, USACE, and DARPA. Potential long-term applications of the research efforts managed within this Program Area include systems that continuously accommodate troop populations of variable size and perform equally well in urban and remote locations under a wide range of climates with maximum recovery of usable energy via physical-chemical and biological processes.

C. Research Investment

The total funds managed by the ARO Environmental Sciences Division for FY10 were $16.4 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $2.5 million. The Defense University Research Instrumentation Program (DURIP) provided $0.7 million to programs managed by the Environmental Sciences Division. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.6 million for projects managed by the Division in FY10. In addition, congressional earmarks provided $1.6 million. Finally, $4.0 million in FY10 was provided by DARPA and $9.2 million was provided by other DoD agencies.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops

1. The 13th Landmine and Explosive Object Detection Review (Washington, DC; 27-28 January 2010). This meeting was organized by the ARO Environmental Sciences Division and hosted by the Catholic University of Washington. It brought together more than 50 people from academia, industry, and DoD organizations, including the National Geospatial-Intelligence Agency (NGA) Space and Missile Defense Command, Joint IED Defeat Organization, ARL Sensors and Electron Devices Directorate (ARL-SEDD), CERDC-NVESD Countermine Directorate, the Office of Naval Research (ONR) Naval Surface Warfare Center and the Naval Academy. The presentations described recent progress and developments for the NGA, and Army- and Navy-sponsored basic and applied research in the broad area of explosive device detection and discrimination and provided an open forum for interactions among principal investigators (PIs) and various laboratories.

2. Military Use of Geothermal Energy (Washington, DC; 23-25 March 2010). The goal of this workshop was to investigate the military use of geothermal energy. The workshop was held at the request of DARPA, and included participation from the Environmental Sciences Division. The objective of this workshop was to ascertain the challenges and opportunities related to the development of geothermal energy at DoD, as well as military bases and installations within the continental U.S. (CONUS) or outside the continental U.S. (OCONUS). Approximately 40 participants from academia, industry, and a variety of federal agencies participated in the workshop.

3. Remote Sensing of Precipitation at Multiple Scales Workshop (Irvine, CA; 15-17 March 2010). This workshop was jointly sponsored by the Atmospheric Sciences and Terrestrial Sciences Programs within the Environmental Sciences Division, and organized by the Center for Hydrometeorology and Remote Sensing, the Department of Civil and Environmental Engineering and the Samueli School of Engineering. The workshop was held at the National Academy Beckman Center on the campus of the University of California at Irvine. The workshop brought together some 50 scientists and researchers from federal agencies, academia, and industry. It explored advanced concepts and the challenges of satellite estimates of precipitation in manners that significantly improve situational awareness and enhance the accuracy, resolution, and communication of precipitation information under various conditions.

4. Review of Microbial Fuel Cell (MFC) Technology and Applications for Wastewater Treatment (Charleston, SC; 15 June 2010). This workshop provided a platform for discussing the potential for applying MFC approaches and related technology to wastewater treatment, with a special emphasis on the waste treatment

needs of the Army. The goals of the meeting were to discuss the waste and water needs of the military as well as its energy requirements in the field, the status of microbial fuel cell technology, and to define the research areas that need to be addressed to advance MFCs so that they may be applied to wastewater treatment.

5. Weather in Mountainous Terrain: Overcoming Scientific Barriers to Weather Support (Tempe, AZ; 1-2 February 2010). Recent Army engagements in mountainous terrain have brought increased attention to mountain meteorology. This workshop was convened to bring together practitioners and scientists to discuss the state of the art of research, to identify scientific and technological barriers to the prediction of mountain weather, and to discuss recommendations for future research directions.

C. Multidisciplinary University Research Initiative (MURI)

No projects were active in FY10.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY10.

E. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY10.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. High-Sensitivity MEMS Biosensor for Monitoring Water Toxicity. The goal of this HBCU project, led by Professor Ioana Voiculescu at The City College of New York, is to characterize endothelial cell responses to toxicants and to test these as a model system for a field-portable toxicity device that is highly sensitive to toxicants in water. The approach is to develop a system with two main parts: (i) a biosensor that will record impedance and resonant frequency measurements from endothelial cells after toxicant exposure and will give information about the cells shape, growth and viability, and (ii) an integrated micro-incubator for the culture of endothelial cells equipped with an automated media delivery system. The system is Army relevant in that the development of a toxicity sensor that can rapidly detect a wide variety of contaminants would be a critical new capability and a significant improvement.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Environmental Sciences Division managed six new DURIP projects, totaling $0.7 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of stable boundary layer dynamics, investigation terrestrial remote sensing, and characterization of complex environments.

I. DARPA Materials with Novel Transport Properties (MANTRA) Program

The ARO Environmental Sciences Division is serving as agent for the DARPA MANTRA program. The goal of this program is to demonstrate a prototype seawater desalination system that produces high rates of potable water from seawater while achieving two orders of magnitude reduction in size and weight and one order of magnitude reduction in power compared to existing systems. The research efforts supported through this program are investigating and designing large-area membranes with substantially reduced defects for improved fluid transport by increasing the use of CNTs or other gatekeeper molecules in the membrane, while preserving the salt rejection at 98%. However, research pursuing evolutionary improvements to the existing state of practice for the rapid development of more advanced membrane concepts is excluded.

J. Global Military Operating Environments: Linking Natural Environments, International Security and Military Operations

The goal of this Congressionally-mandated project is to explore military testing and training in support of the Army Yuma Proving Ground Natural Environments Test Office. Five distinct research efforts are being pursued: (i) Multiple Master Environmental Reference Sites (MERS) for comprehensive characterization of soil processes will be established at sites that represent prevalent terrain conditions critical for military operations and testing (*i.e.*, different military operating environments; MOE), (ii) data analysis of the established MERS will be initiated to evaluate the temporal dynamics of energy fluxes under both natural and disturbed conditions in different climatic regimes, (iii) techniques and methods will of incorporating data on soil and soil surface processes and conditions in the development and testing of technologies for the detection and defeat of IEDs will be studied and a set of recommended approaches developed, (iv) terrain conditions at primary testing and training installations will be characterized to determine terrain analogs for areas of current and future strategic interest, and (v) a military environments reference database will be created that compiles soil and terrain data and related literature to increase availability of global terrain data to the testing and training community. The research proposed is directly relevant to the Army's test and evaluation mission and has extremely high relevance to Army requirements gaps and material technical shortcomings. Providing better insight and understanding of actual military operating environments worldwide to the Army test community will lead to improvements in test procedures and methodologies for Army materiel and systems and aid in improving the performance of sensors and multi-sensor systems used for explosives detection.

K. Multi-Sensor Detection of Obscured and Buried Objects Program

This program is sponsored by CERDEC-NVESD, Countermine Division and the goal is to develop new algorithmic approaches for detecting obscured and buried objects using multi-sensor systems. The research will primarily explore systems that use some combination of Ground Penetrating Radars (GPR), Electro-Magnetic Induction (EMI) sensors, and Electro-Optical (EO) Systems, including broad-band cameras, as well as multi- and hyper-spectral imaging systems. A broad program of signal processing research that focuses on the development and enhancement of feature-extraction and classification algorithms will be pursued. In the area of GPR, the effort will investigate, develop, and test Hidden Markov Model discrimination algorithms based on Gabor features. The utility of using differential data-driven and model-based techniques to process Argand diagrams of wideband EMI systems will be investigated. The use of a random set method for providing context-based cueing from an airborne multi- or hyper-spectral system to a ground-based GPR or GPR/EMI system will be explored. The use of Bayesian methods for combining multiple experts as a means of accommodating strengths and weaknesses of different sensors will be studied. Finally, modeling class preference relations for rank-based fusion will be investigated. The work to be undertaken is highly relevant to current Army countermine and explosive object detection programs at CERDEC-NVESD, all of which have a critical need for advanced signal processing algorithms.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Environmental Sciences Division.

A. Geo-Spatial Enabled Dynamic Network Analysis

Professor Kathleen Carley, Carnegie Mellon University, Single Investigator Award

The objective of this project is to combine dynamic social network data with spatial information to ultimately develop tools for data assessment using both dynamic social network analysis and geospatial analysis. This goal is being pursued using the social network analysis tool Organizational Risk Analyzer (ORA) for assessing meta-network data (see FIGURE 1). The investigator has developed a theory of social and knowledge networks that is geospatially-enabled and constrained. This new theory is leading to an improved understanding of the technology, algorithms, and metrics needed to assess and visualize data that contains both geospatial and network information, as a basis for theory examination and validation. The investigator utilized this theory to explore how the inclusion of geospatial constraints alter the predictions of dynamic network models and whether the inclusion of such information increases prediction accuracy.

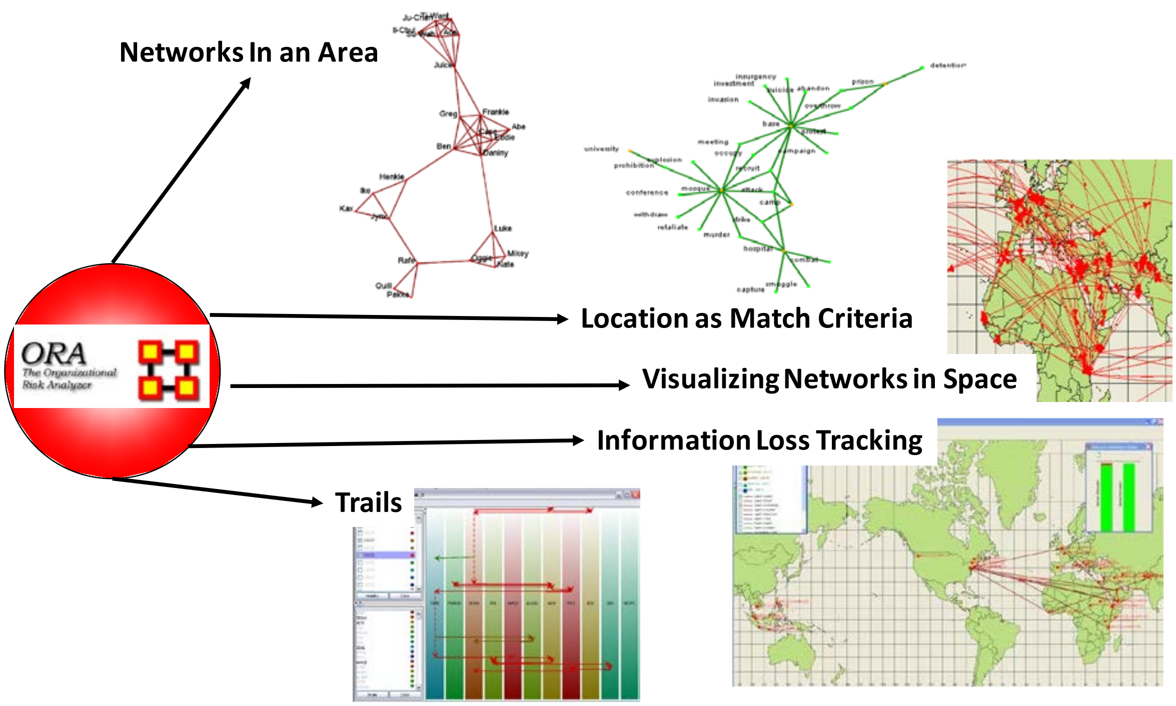

FIGURE 1

Organizational risk analyzer (ORA). The diagram illustrates the components involved in the ORA process for geo-spatial network analysis.

B. Dry Snow Metamorphism

Professor Ian Baker, Dartmouth College, Single Investigator Award

The goal of this research is to analyze and characterize the structural evolution of dry snow as it undergoes metamorphism under either quasi-isothermal conditions or a temperature gradient, and to determine the dominant mass transport mechanism. The effect of a temperature gradient on the sintering of ice crystals was explored and structural evolution and the changes in structural parameters, such as density, specific surface area, and degree of anisotropy were measured. The observational techniques being used in this project involve a combination of optical microscopy, scanning electron microscopy (SEM) and X-ray computed microtomography

(micro-CT). Because of its non-destructive nature, micro-CT has enabled the collection of time-series images, including the acquisition of various quantified structural parameters as porosity and specific surface area. Fine structural features and impurities in both fresh and metamorphosed (*i.e.*, sublimated) snow were characterized using SEM (see FIGURE 2). Finally, a mathematical model was formulated for describing and understanding the behavior of snow during metamorphism and grain sintering.

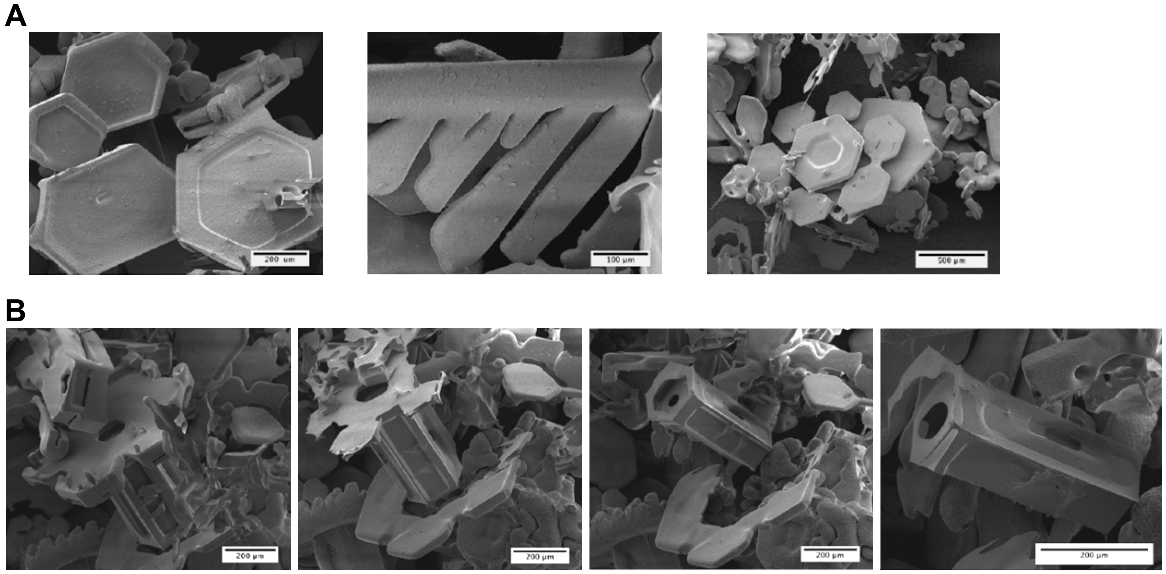

FIGURE 2

Fresh and metamorphosed snow analyzed by SEM. (A) These images are secondary electron micrographs of a freshly-fallen snow specimen collected during a snowfall in Hanover, New Hampshire. The snow specimen was maintained at -180ºC to avoid sublimation. As shown in the image, the snow specimen encompassed a variety of morphologies, however, the majority were flat hexagonal plates with narrow grooves frequently appearing on their edges. (B) These secondary electron images reveal the sublimation-induced structural changes of a snow crystal under high-vacuum conditions in the SEM chamber. The temperature was increased from -180°C (left-most image) to -100°C (right-most image) over 25 minutes; the accelerating voltage was 2 kV.

C. Studying Multiscale Phenomena in the Solid-Liquid Transition State of a Granular Material

Professor R. Behringer Duke University, Single Investigator Award

Professor R. Behringer at Duke University and Professor A. Tordesillas at the University of Melbourne in Australia, are collaborating to explore the loading behavior of granular materials near the liquid-solid (jamming) state. Using unique experimental facilities at Duke University, a series of slider/friction experiments were recently completed using photoelastic particles subjected to dynamic deformation to produce unique information on granular slip and friction (see FIGURE 3).

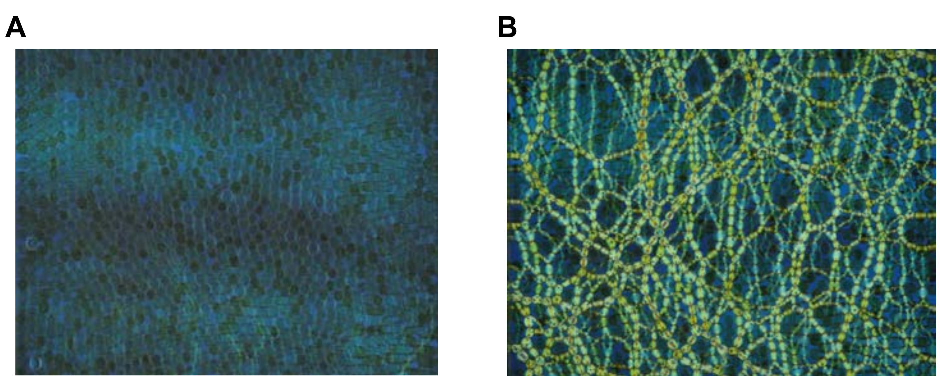

FIGURE 3

2D granular slip experiment using photoelastic particles. (A) The initial state reveals isotropic stress distribution, while the (B) final state with large stress following a shear cycle reveals jammed particles and the development of force chains.

In one set of experiments, an object was pulled across the surface of a layer of photoelastic particles. Simultaneous measurements were made of the pulling force and the photoelastic response of the granular layer. It was then possible to correlate the slipping behavior of the object to the internal response of the granular material. These experiments will allow for the detailed determination, at the particle level, of all physically relevant properties of a model granular system subjected to dynamic loading. Specifically measurements are made of displacement, rotation, and all contact forces for every particle in the loaded system. This accomplishment provides an approach for obtaining experimental information at all scales within a granular material. From these properties, it is possible to compute stresses and other quantities that are relevant at the macroscopic scale. The experimental data show that granular materials fail under traction by a process that dissipates energy relatively deeply into the material. These data detail the nature of granular slip and ultimately may suggest ways to maximize traction/avoid slip under a vehicle.

A second set of experiments focused on the multiscale nature of failure under shear, which is arguably the most important failure mode for granular materials subjected to dynamic loading. In this case, the experiments again exploited the special properties of photoelastic particles. The particles are contained in a biaxial device whose purpose is to provide highly controlled shear. Data was generated for particle properties, contact forces, particle displacements and macroscopic properties (*e.g.*, stresses). A particularly interesting recent finding from this work is the observation that weak granular materials, such as loosely packed unstable soils, can be stabilized (*i.e.*, jammed or become solid-like) by the application of shear. This result will require a significant rethinking of current models of particle jamming. A new description is being developed for the localized deformation leading to failure using highly novel topological and network approaches. This experimental research conducted at Duke University was closely coordinated with theoretical modeling and discrete-element modeling studies at the University of Melbourne.

This collaborative basic research in granular materials will continue to provide USACE with new micromechanical constitutive models of dry granular materials that, after experimental validation, will provide a computationally efficient alternative to discrete element simulations and fill an important niche in soil-structure/machine interaction systems modeling beyond the reach of current capabilities.

D. Investigating the Impact of Dike Structures on Sediment Transport in Alluvial Rivers

Professor G. Duan, University of Arizona, Single Investigator Award

This research is exploring turbulent flow and sediment transport in meandering rivers and in rivers near dike structures of various geometries, through an integrated program of laboratory experiments, numerical modeling, and field application. A set of experiments was conducted at the hydraulics laboratory at the University of Arizona with discharges representing low flow stage, a 2-year flow event, and a 5-year flow event scaled based on field observations. For each discharge, several experimental runs for different dike alignments were tested. Sediment-laden flow with a specified hydrograph was released at the inlet with a sluice gate used to control water surface elevation at the outlet. The experimental results were modeled numerically using *EnSed2D*, an enhanced 2D sediment transport model that solves the depth-averaged Reynolds approximation of Navier-Stokes equations to obtain depth-averaged horizontal velocities (see FIGURE 4).

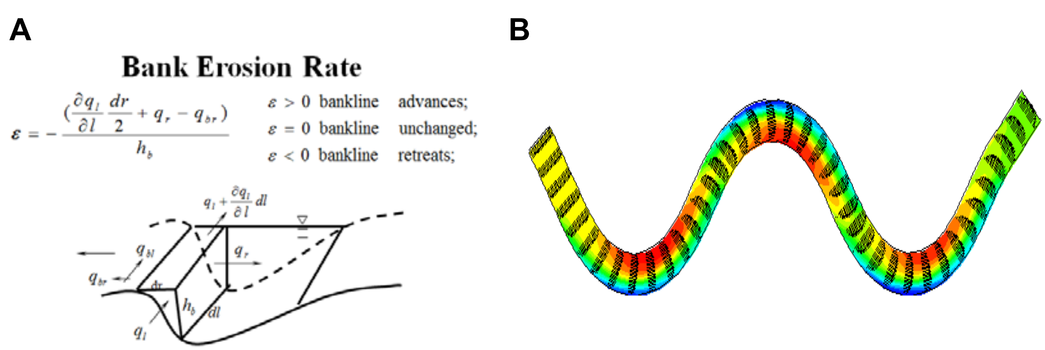

FIGURE 4

Model of bank erosion rate. (A) A sediment model was used to calculate the flow velocity field, (B) shown with color denoting bed elevation and vectors the flow velocity for a meandering river.

The flow depth and concentration of suspended sediment were obtained by solving the continuity equations for suspended sediment-laden flow and suspended solids, respectively. The dispersion terms derived from the linear approximations of longitudinal and transverse velocity profiles were included in the momentum equations to account for the secondary flow. For the field component of the study, the model was applied to the left bank immediately upstream of Huron Island at River Mile 425 on the Mississippi River. The total length of the study reach was about 17 miles. The uncertain parameters in hydrodynamic and sediment model are turbulent eddy viscosity, bed roughness, bed load transport rate, and suspended sediment concentration. The EnSed2D model will be verified in subsequent studies using the experimental data, as the uncertainties of these data obtained from field survey could significantly affect the accuracy and reliability of the modeling results.

E. Human Cognition and Optical Remote Sensing for Disturbed Soil Recognition

Professor J. Staszewski, Carnegie Mellon University, Single Investigator Award

This research effort is bringing together two disparate disciplines: human cognition and optical remote sensing, to create new fundamental knowledge and understanding about how optically-available terrestrial information is perceived and used by human experts in tactical tracking. The objective of this project is to quantify, systematize, augment, and ultimately automate the tracking of small-scale human movement within deserts and other poorly vegetated, environments. The effort is describing in detail, both qualitatively as well as quantitatively, the optical information resulting from disturbance of ground by human movement and the manner in which information capable of supporting tracking, changes as a function of time and environmental exposure. The physical and mineralogical effects of disturbance, both immediate effects and the aging of these effects, are being characterized. The extent of the use of photometric techniques is being investigated, including characterizing enhanced backscatter and polarization from visible to shortwave infrared wavelengths.

The investigator recently demonstrated the use of thermal and reflected illumination techniques, such as light detection and ranging (LIDAR), for characterizing and quantifying surface roughness (see FIGURE 5). LIDAR is an optical remote-sensing technology that measures scattered light properties to find the range of a distant target.

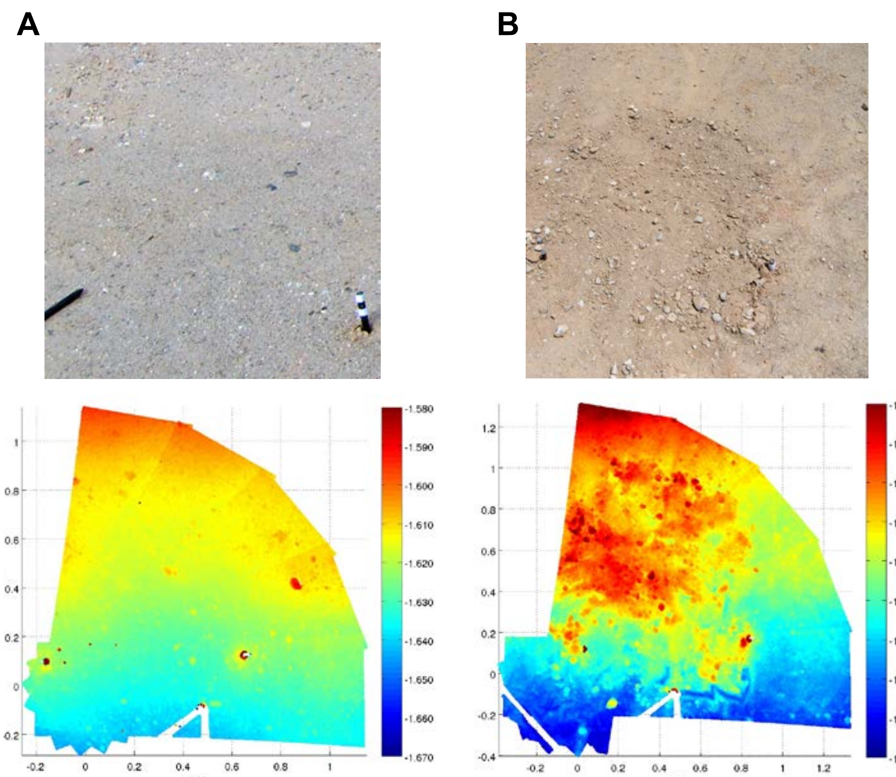

FIGURE 5

Surface roughness analysis. The optical images and LIDAR scans are of (A) undisturbed and (B) disturbed desert soil.

F. Optimization of Electrocoagulation and Coagulation Pretreatment for Ultrafiltration

Professor Brian Dempsey, Pennsylvania State University, Single Investigator Award

The goal of this project is to explore the use of in-line electrocoagulation as a pretreatment for seawater prior to ultrafiltration at the bench-scale. The investigator evaluated ultrafiltration membrane performance by measuring trans-membrane pressure (TMP) and hydraulic resistances at sub- and super-critical fluxes, and assessed flux recovery after hydraulic and chemical cleanings. They discovered that compared to no coagulant pretreatment, ferric chloride improved ultrafiltration membrane performance under short-term, constant flux conditions resulted when trans-membrane pressure was <8 psi, but produced increased resistance to filtration above 15 psi. In addition, the research team found that electrocoagulation consistently resulted in lower resistance and improved flux recovery compared to an equivalent dose of ferric chloride (see FIGURE 6). Based on these results, the investigator noted that electrocoagulation may be a feasible and competitive pretreatment strategy in the laboratory. In the longer term, various scale-up considerations such as electrode cleaning requirements and sustainability over long-term operation will be assessed.

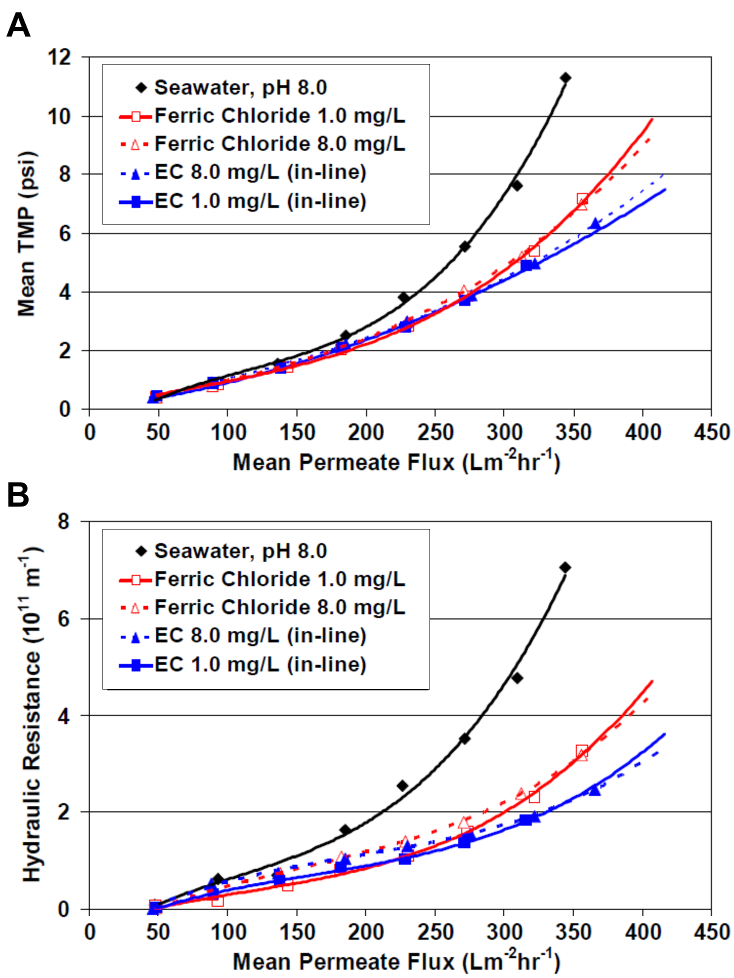

FIGURE 6

Electrocoagulation lowers resistance and improves flux recovery relative to ferric chloride. The resulting (**A**) transmembrane pressure (TMP) and (**B**) hydraulic resistance were assessed with seawater samples pretreated with ferric chloride or electrocoagulation (EC); doses are reported as mg/L as Fe.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Systematic Approaches for Calibration of Subsurface Transport Models

Investigator: T. Illangasekare, Colorado School of Mines, Single Investigator Award
Recipient: USACE-ERDC Countermine Testbed Program

Researchers at the Colorado School of Mines (CSM), led by Professor Illangasekare, have provided USACE-ERDC with experimental data sets on the temporal and spatial distribution of soil moisture and temperature in the shallow subsurface environment that can be used to better understand fundamental processes and validate numerical models. For the past five years, the ERDC Countermine Testbed program has been testing automated target recognition software (ATRs) on synthetic IR imagery to increase the accuracy of landmine detection and reduce false alarms. The research has focused on generating synthetic IR images which are added as test cases for ATR software. The production of synthetic imagery allows for a variety of scenarios to be tested that would be costly or difficult to test in the field.

Because landmine sensors exploit soil and environmental conditions to discern between mines and other objects, most mine detection technologies require that the spatial and temporal variability of key environmental conditions such as climate, vegetation, soil type, depth of ground water table, and topography be understood. If these factors and the ability to model them in a variety of domains become well defined, then sensor and algorithm simulations can more realistically be tailored to particular operational scenarios and technologies.

The experimental data sets provided by CSM represent a systematic experimental study of the effects of the near surface boundary conditions on soil moisture and temperature distributions in the shallow subsurface. Increased knowledge of the effects of geohydrologic/thermal properties and behaviors on the landmine signature will ultimately help to properly interpret sensor imagery. In addition, these data will be used to validate and improve calculations from ERDC's Computational Testbed.

B. Multiscale Phenomena in the Solid-Liquid Transition State of a Granular Material

Investigator: A. Tordesillas, University of Melbourne, Australia, Single Investigator Award
Recipient: USACE-ERDC Geotechnical and Structures Laboratory

Forces in a deforming granular medium are transmitted in a dual-particle network. This network involves the so-called "strong network," comprising nearly linear particle chains (also known as "force chains") which bear above-the-global-average loads or forces, and the complementary "weak network" which surrounds the strong network, comprised of particles that bear below-the-global-average loads. Force chains form one of the basic building blocks of dense granular systems; therefore, their accurate identification has obvious significance in understanding the behavior of these systems. The development of robust predictive tools to investigate thermo-micro-mechanical continuum theories of shear banding and comminution phenomena in particulate systems crucially depend on accurate knowledge of force chains and their evolution during deformation.

Professor Tordesillas, head of the Mechanics of Granular Media Group at the University of Melbourne, Australia, has transitioned a new particulate mechanics modeling code, *Forcechain3D*, to the USACE-ERDC Geotechnical and Structures Laboratory. The *Forcechain3D* code determines the force chains and, hence the strong and weak network in a 3D assembly of particles of arbitrary shape. This code, while designed for granular systems, may have broader utility. Other forms of complex matter, such as colloids and other nanoparticles, are also known to exhibit similar structures. Therefore, tools of this kind may also prove useful in the characterization of force transmission in such systems.

C. Geospatial Enabled Dynamic Network Analysis
Investigator: Kathleen Carley, Carnegie Mellon University, Single Investigator Award
Recipients: Army Training and Doctrine Command (TRADOC) and the FBI

Professor Carley and her research group at the Center for Computational Analysis of Social and Organizational Systems (CASOS) have been studying the complexity of socio-technical systems. Recently CASOS began transitioning the capabilities of its ORA, a risk assessment tool for locating individuals or groups that are potential risks given social, knowledge and task network information, to government security and law enforcement agencies within and outside DoD (refer to Section III: *Scientific Accomplishments)*. ORA links geospatial and network analytics to identify key actors based on movement and asses shifts of groups in different geographic regions thus providing critical information for planning facilitating tactical missions. As part of this outreach and transition process, Professor Carley has trained a number of government groups in how to use ORA and the new geo-spatial network tools that are now incorporated into ORA. During the past year, representatives from multiple agencies received ORA training, including TRADOC and the International Gangs Unit of the FBI.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Physics-Based Modeling of Bridge Foundation Scour

Professor Panos Diplas, Virginia Polytechnic Institute and State University (Virginia Tech)

This research is being conducted collaboratively by Virginia Tech, the St. Anthony Falls Laboratory of the University of Minnesota, and the USACE-ERDC Waterways Experiment Station. This effort is jointly funded by ARO and the National Science Foundation Hydrologic Sciences Program. The objective of this project is to develop and validate the first 3D unsteady state numerical model capable of accurately producing bridge foundation scour. This research project will integrate the latest developments in the numerical modeling capable of resolving 3D coherent hydrodynamic structures of turbulent juncture flows with state-of-the art laboratory experimentation in which simultaneous measurements are made of instantaneous flow quantities and pressures within the progressive spatial and temporal development of a scour hole.

It is anticipated that in FY11 the collaborative research team will design and perform scour experiments with erodible boundary, design and implement an image analysis methodology using time-resolved digital stereo particle image velocimetry and acoustic dopplar velocimetry, and perform experiments intended to resolve the real-time scour hole evolution COE-ERDC Large-Scale Sediment Transport Facility.

B. Impact of Dike Structures on Sediment Transport in Alluvial Rivers

Professor G. Duan, University of Arizona

This research is exploring turbulent flow and sediment transport in meandering rivers and in rivers near dike structures of various geometries, through an integrated program of laboratory experiments, numerical modeling, and field application. It is anticipated that in FY11, the final year of this project, this research effort will have completed a panel of experimental data for model verification, the modification and validation of the EnSed2D sub-model for simulating the alluvial processes of river bed degradation/aggradation and bank erosion, and will have performed risk and parameter uncertainty analysis of modeling results affecting the predictions. The long-term result of this research may be a feasible design of dike structures for bank protection and ecosystem restoration that can effectively reduce sediment deposition and maintain a favorable flow condition during winter low flows in the island.

C. Effects of Stability, Canopies, and Non-Stationarity on Dispersion in the Stable Boundary Layer

Professor Jeffery Weil, University of Colorado, Boulder

The the goal of this project is to simulate more stable, time-varying, and possibly intermittent SBLs than have been achieved previously using large eddy simulations (LES). These simulations are being pursued through a collaboration with Drs. Edward Patton and Peter Sullivan at the National Center for Atmospheric Research. The dispersion and concentration fields due to a scalar source are obtained by tracking “passive” particles with a Lagrangian particle dispersion model (LPDM) driven by velocity fields from the LES. The dispersion calculations are focused on the mean concentration fields, plume dispersion statistics, and the statistical variability in concentration due to continuous point sources.

Significant progress has already been made in developing the quasi normal scale elimination approach for turbulent closure in stably stratified (nocturnal) boundary layers and incorporating it into the Weather Research and Forecasting model used by Air Force Weather Agency and the atmospheric sciences community for operational and research forecasting. A weakly unstable form of quasi normal scale elimination was developed, but had limited applicability. In unstable cases (daytime), the closure reverted back to the conventional closure, causing a mismatch of physics. Initial results in canonical cases indicate reduced bias and root mean square

error to provide better estimates of boundary layer heights and smooth transitions between stability regimes. In the coming year, further inter-comparisons with field data over diurnal periods will be evaluated, and regional forecast evaluations will follow in preparation for weather research and forecasting inclusion.

D. Ordered Molecular Transporters
Professor Bruce Hinds, University of Kentucky

The goal of this project is to determine if and to what extent a new class of nanoscale devices can be designed with greatly improved efficiency to selectively transport gasses and fluids at very high rates. The research pursues new opportunities for the templated growth of carbon nanotubes with molecularly controlled diameters and molecular net crown ether gatekeepers for single file water flow at dramatic rates. It is anticipated that in FY11 the effort will lead to the development of a new single-walled carbon nanotube design with the ability to perform ion separation from water.

VI. DIVISION STAFF

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Program Manager, Atmospheric Science

Dr. Russell Harmon
Program Manager, Terrestrial Sciences

Dr. Larry Russell
Program Manager, Multidisciplinary University Research Initiative Program

Ms. Sandra Elizondo
Directorate Secretary

Mr. William Cheek
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Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 7: LIFE SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Life Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research efforts to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes governing DNA, RNA, molecular and genetic systems, proteins, organelles, prokaryotic cells, eukaryotic cells, unicellular organisms, multicellular organisms, multi-species interactions, individual humans, and groups of humans. More specifically, the Division aims to promote basic research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and possible non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics & host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of research in the life sciences. In addition, these efforts will likely reveal new methods for protecting the Soldier and optimizing warfighter performance capabilities.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of biological processes, the research efforts managed by the Life Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the discoveries uncovered by ARO in the life sciences may provide new technologies for protecting the Soldier, for maintaining and improving warfighter mental and physical performance capabilities, for creating new biomaterials, and for new advances in synthetic biology for energy production, intelligence, and bioengineering.

3. Coordination with Other Divisions and Agencies. To effectively meet Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division frequently coordinates and leverages efforts within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Joint Improvised Explosive Device Defeat Organization (JIEDDO), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the Center for Disease Control (CDC), the National Institute of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO and ARL Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of

research approaches. For example, interactions with the ARO Chemical Sciences Division include promoting research to understand abiotic/biotic interfaces. The Life Sciences Division also coordinates efforts with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics. In addition the Division coordinates with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Life Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these five Program Areas: (i) Genetics, (ii) Neurosciences, (iii) Social and Behavioral Science, (iv) Biochemistry, and (v) Microbiology and Biodegradation. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The goal of this Program Area is to understand and characterize gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration. Research is expected to lead to new avenues for reducing Soldier mortality and for improving Soldier physical and mental performance capabilities. This Program Area is divided into two research Thrusts: (i) Soldier Performance, and (ii) Soldier Protection. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research efforts within these Thrusts investigate human performance and protection under normal conditions and when affected by a variety of stressors that are likely to be encountered in battlefield situations, such as dehydration, heat, cold, sleep deprivation, fatigue, caloric insufficiency, microbial factors, and psychological stress. Potential long-term effects on the Army include improved Soldier performance, the ability to maintain Soldier performance at peak capacity when needed, a reduction in cognitive errors, better integration of machines and technology with the human brain, new sources of energy production, and new biomaterials for Soldier protection.

2. Neurosciences. This objective of this Program Area is to use non-medically oriented research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and possible non-invasive methods of monitoring cognitive states and processes during normal activity. The research areas include perceptual and/or psycho-physiological implications of mind-machine interfaces ranging from optimizing auditory, visual and/or somatosensory display and control systems based on physiological or psychological states through modeling of individual cognitive dynamics and decision making. This Program Area is divided into two research Thrusts: (i) Neuroergonomics, and (ii) Neuromorphics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Neuroergonomics Thrust aims to understand how the human brain functions in relation to sensory, cognitive and motor processes during its performance in real-world tasks in order to develop. Research in the Neuromorphics Thrust is focused on understanding how individual neurons, circuits, and overall architectures create desirable computations, affect how information is represented, influence robustness to damage, incorporate learning and development, and facilitate evolutionary change. Cell culture and social insect models are being used to develop better understanding of living neural networks and swarm intelligence for eventual application in Army systems.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications, current research may ultimately enable the development of neural biofeedback mechanisms to sharpen and differentiate brain states for possible direct brain-machine communication and to determine how closely humans can approach hemispheric sleep as seen in some migrating birds and in dolphins.

3. Social and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior through the development of mathematical, computational, statistical, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics

(see FIGURE 1). This Program Area is divided into two research Thrusts: (i) Predicting Human Behavior, and (ii) Complex Human Social Systems. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. The program supports scientific research that focuses on the basic theoretical foundations of human behavior at various levels (individual actors to whole societies) and across various temporal and spatial scales. This includes, but is not limited to, research on the evolution and dynamics of social systems and organizations, human adaptation and response to both natural and human induced perturbations (*e.g.*, global climate change, mass migration, war, attempts at democratization), interactions between human and natural systems, the role of culture and cognition in accounting for variations in human behavior, human decision-making under risk and uncertainty, the search for organizing principles in social networks, and the emergent and latent properties of dynamic social systems and networks. The research involves a wide range of approaches, including computational modeling, mathematical modeling, agent-based simulations, econometric modeling and statistical modeling, to name a few. The program also recognizes the fact that the building and validation of models in the social sciences is often limited by the availability of adequate and appropriate sources of primary data. Thus some of the supported research includes the collection of primary data for the development and testing of models. Finally the program also supports research in the development of methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that have the potential to help advance our scientific understanding of human behavior.

Research focuses on high-risk approaches involving highly complex scientific problems in the social sciences. Despite these risks, the research has the potential to make significant contributions to the Army through applications that will, for example, improve decision-making at various levels (policy, combat operations), create real-time computer based cultural situational awareness systems for tactical decision-making, increase the predictability of adversarial intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

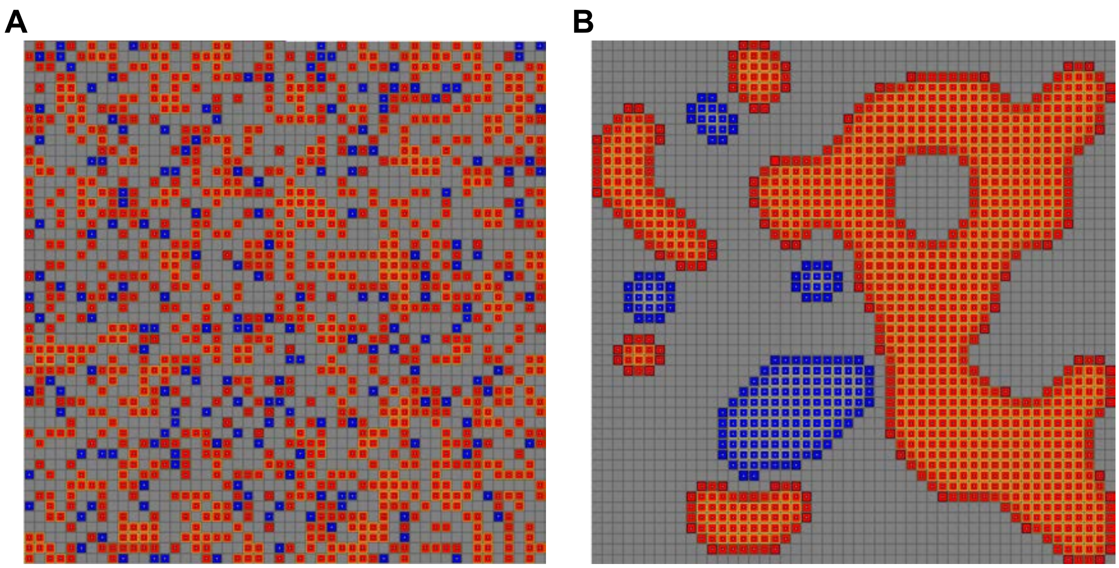


FIGURE 1

Simulation of socio-cultural dynamics. The figure illustrates the results of a cultural agent-based model with two cultures, simulating the evolution of subgroup formations under (**A**) moderately-positive attitudes towards in-group members and (**B**) negative attitudes towards out-group members.

4. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. Research in this program may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules. This Program Area supports two research Thrusts: (i) Biomolecular Function and Engineering, and (ii) Biomolecular Structure and Assembly. Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the Biomolecular Function and Engineering Thrust aim to understand and control biomolecular activity, to identify the determinants of the specificity of molecular recognition and modulate this specificity through protein engineering, and to improve

the stability and purity of biomolecules for utilization in nanoscale engineered systems. Research in the Biomolecular Structure and Assembly Thrust aims to explore the fundamental principles governing biological self-assembly, and to understand and control the interactions and forces operating at the interface between biological molecules and abiological materials.

The basic research efforts supported by this program promote potential long-term applications for the Army that include biosensing platforms that incorporate the exquisite specificity of biomolecular recognition, nanoscale biomechanical devices powered by motor proteins, novel biotic/abiotic materials endowed with the unique functionality of biomolecules, drug delivery systems targeted by the activity and specificity of biomolecules, electronic and optical templates patterned at the nanoscale through biomolecular self-assembly, and novel power and energy systems that utilize biomolecular reaction cascades.

5. Microbiology and Biodegradation (MBD). This Program Area focuses on understanding microbial physiology, genetics, ecology and evolution. Microbes are distributed throughout nature and are, in fact, essential for all life; however, microbes can also cause problems ranging from catalyzing materiel degradation to life-threatening infections. Therefore understanding how these organisms thrive and adapt to various environmental niches, and how they adapt to new environments, is of great importance. This Program Area is divided into two research Thrusts: (i) Microbial Growth and Viability, and (ii) Biodegredation, Bioenergy, and Biomaterials. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Included in this program are studies to understand antimicrobial resistance mechanisms; microbial community interactions; microbial evolution, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell level or in mixed populations (*e.g.*, metagenomic); and studies of organisms that have adapted to grow or survive in extreme environments. Also included is research on biochemical and physiological mechanisms underlying biodegradation processes in normal, extreme, and engineered environments; studies of microbiological mechanisms with potential for contributing to the remediation of sites contaminated with toxic wastes; and the development and exploitation of microbial systems for unique biotechnological applications and bioengineering processes.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include strategies for harnessing microbes to produce novel materials, protect materiel, and efficiently produce desirable commodities; innovative strategies for controlling bacterial infections and preventing or treating infectious diseases will also be enabled.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY10 were $104 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $4.7 million. The DoD Multi-disciplinary University Research Initiative (MURI), and Defense University Research Instrumentation Program (DURIP) provided $2.8 million and $1.2 million, respectively, to programs managed by the Division. The Division managed $54.2 million provided by the Defense Advanced Research projects Agency (DARPA), and $19.2 million provided by other agencies, including DTRA, JIEDDO, MRMC, NSRDEC and the Army Special Operations Command (SOCOM). The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $2.3 million for awards in FY10. In addition, congressional earmarks provided $3.6 million. The Institute for Collaborative Biotechnologies received $9 million in FY10. Finally, $0.4 million in FY10 was provided for the Presidential Early Career Award for Scientists and Engineers (PECASE) program and $0.6 million for the Historically Black Colleges and Universities (HBCU) outreach program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. 2010 Beyond Brain Machine Interface Workshop: From Senses to Cognition (Long Beach, CA; 20 June 2010). This workshop was designed to push the frontiers of research related to a future Brain Machine Interface (BMI) from the sensory and motor interface to enhancing cognitive and physical performance. The workshop laid the groundwork for the neuroscience, technology, and clinical translations by bringing scientists from around the world together to present the state of the art and discuss future directions. The conference led to the design of a roadmap that lays out the research and potential funding vehicles (*e.g.*, SBIR/STTR) that may enable the research to move from basic to applied technologies.

2. DoD Biosensing Task Force (Republic of Mozambique; 20-28 July 2010). It is expected that enemy forces will increasingly move to the use of plastic cased non-metallic mines and improvised explosive devices (IEDs). This necessitates the use of detection systems that are not metal-based. Direct smelling of explosive vapor is done either by explosive trace detector equipment or with animals. Although not rigorously quantified, it is apparent that trained animals are capable of detecting explosives at levels lower than abiotic systems, such as gas chromatography, mass spectrometry (GC/MS). A task force of de-mining experts was assembled to investigate the reported mine-detecting abilities of giant African pouched rats to determine whether the rat has potential utility for the U.S. in de-mining operations (see FIGURE 2).

FIGURE 2

African giant pouched rat searching for mines in various east African countries. The DoD Biosensing Task Force meeting in July 2010 discussed studies of this rat for mine detection.

A team of experienced de-miners, trainers for explosives-detecting canines, biochemists, a combat engineer, a rodent behavior expert, and a veterinarian traveled to Mozambique and Tanzania to first hand observe and evaluate the rat based mine detecting operations done by APOPO, a Belgium-based non-profit de-mining group. This group confirmed that the African giant pouched rat has the ability to detect land mines. Despite their small size, these rodents possess an alert signal that, if reinforced with improved training of both the pouched rat and the handlers, can be a powerful tool. The time required to train the pouched rats is comparable to that for dogs, and the current cost of producing an accredited mine detecting rat is lower than a comparably accredited dog, primarily due to the lower cost of labor in east Africa. Compared to dogs, pouched rats appear to have simpler logistical needs, potentially making them an economical alternative to the use of dogs in selected situations. Small animal based detection systems also have potential value in exploring spaces too small for people to get into or that are otherwise difficult for humans or dogs to access. In addition, warfighters could carry rats in their backpack, they would be more covert than dogs, and could be left behind at the end of the mission. Other uses that could be explored include detecting weapons caches and IEDs.

Although APOPO demonstrated that approximately twenty African giant pouched rats detected over 500 mines in an area approximately 5 kilometers by 100 meters with minimal technological support over ten months, the precise detection capability as well as the false negative rate remains poorly substantiated. Independent validation is planned to more precisely quantify the explosive detection sensitivity and accuracy of rats.

3. Bio-Directed Assembly Basic Research Workshop (Keystone, CO; 18-19 May 2010). Nature has evolved methods to assemble biological molecules with exquisite control, generating intricate assemblies on the nanoscale. These assembly processes could be exploited for the next generation of nanoscale fabrication technologies for materials, electronics, optics, and power systems. The goal of this workshop was to bring together key researchers at the forefront of the field of bio-directed assembly to discuss recent advances in the field and identify key knowledge gaps and potential research directions. The workshop led to a discussion of new scientific opportunities that could address current barriers in the field. This workshop brought together experts from academia and government to discuss recent advances in computational design of assembly architectures, techniques for physical assembly of bio-architectures, and technologies for characterization and visualization of assemblies.

4. Computational Biology Training and Workshop (Berkeley, CA; 9-12 August 2010). The goal of this joint Life Sciences and Mathematical Sciences Division sponsored Training and Workshop was to introduce computational biology to DoD researchers and to discuss new needs in the fundamental research area of computational biology. Advances in biotechnology, such as genome sequencing, proteomics, metabolomics and transcriptomics, have led to an explosion of data characterizing biological systems. As the amount of such information grows exponentially, novel methods of data analysis and data interpretation are needed in order to optimally exploit this rich data collection. The two day "Crash Course in Systems Biology" training familiarized primarily biological researchers with current computational biology software and capabilities, with an emphasis on quantitative applications for understanding and modeling complex biological systems. The subsequent two-day workshop brought together leaders in the field from academic and government laboratories to present the state-of-the-art in three areas: (i) experimental inference of growth requirements and interactions of environmental microbes *in situ*, (ii) enrichment and analysis of environmental microbes for laboratory study, and (iii) computational prediction of growth conditions and composition. The workshop presentations were followed by a discussion of the fundamental research needed to revolutionize our ability to perform efficient microbial data integration, and eventually lead to an automated data processing system capable of microbial forensics analyses, among other applications of Army interest.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Characterizing Interfaces between Living and Non-living Structures. This MURI began in FY06 and was awarded to a team led by Professor Paul Cederna at the University of Michigan. The goal of this research is to investigate the neurological and physiological connections required for the normal function of appendages.

The long-term goal of this research is to uncover the materials and methods required to establish functional and structural connections between living limb segments and nonliving devices. The MURI team is exploring the interface between living and non-living structures, including bone, skin, muscle and nerve. Setting prosthetic materials research on a firm theoretical foundation, based in physiological interfaces and principles, will enable the current art of anatomical and physiological compensation to be set on a scientific rather than an empirical foundation. In FY09, the research team developed a method for directly connecting with peripheral nerves, using a soft, electrically conductive scaffold that can be filled with muscle cells to act as targets for propagating axons (see FIGURE 3). As a result of these data, the research has led to a spin-off project currently being considered for separate funding in order to advance the state of knowledge to the point of clinical trials. The ability to design and build intelligent, adaptive, active devices using such engineered biological/non-biological interfaces could ultimately permit a complete return to duty for military personnel with no diminution of ability as well as producing a seamless body of knowledge allowing augmentation of limited function to normal or even enhanced levels of performance.

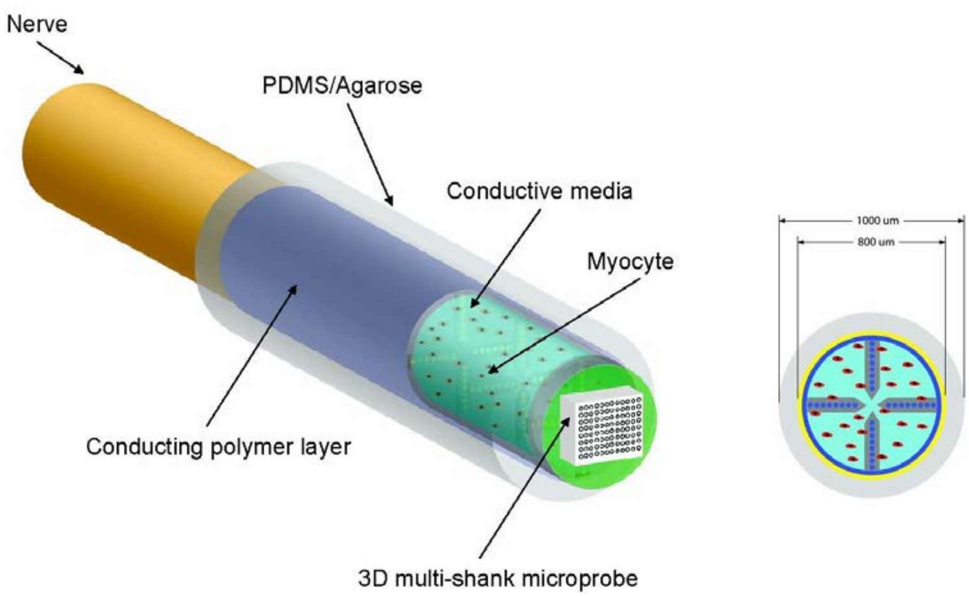


FIGURE 3

Artificial neuromuscular implants (ANMI). Proposed signal interface between a living nerve and an electronic recording system using conductive polymers and cultured muscles cells (myocytes).

2. Exploring Brain-to-muscle Neural Signaling. This MURI began in FY08 and was awarded to a team led by Professor Thomas D'Zmura at the University of California, Irvine. The objective of this research is to investigate brain signals and the corresponding muscle responses.

This team is using electroencephalographic (EEG) readings of brain, which measure electrical activity along the scalp produced by the firing of brain neurons, to determine whether thought (*i.e.,* unspoken) words can be decoded. The MURI leverages breakthroughs in neuroscience and cognitive science uncovered in recent years. These breakthroughs, when coupled with technological advances in both hardware and software, have significantly advanced research progress that may ultimately lead to brain-computer interfaces (BCIs) that can decode the activity in brain networks. This potential long-term application is nearly analogous to the development of speech recognition software; however rather than having sound as the input, the inputs will be EEG signals. This concerted research effort will also attempt to develop a computational model that could decode intended mental speech and decode the direction of the attentional orientation of an individual based solely upon recorded activity from the surface of the scalp.

Preliminary results from the research teams have revealed that the EEG can be used to detect imagined speech rhythm and that the pattern of stress in auditory imagery generated by imagined speech. Results from studies of attentional direction have suggested that covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas activated as part of motor planning for physical orienting (see FIGURE 4). EEG signals generated during lateralized covert attention resemble strongly those used in conventional BCIs to signal left and right through lateralized motor imagery.

Additional results using magnetoencephalography (MEG; a non-invasive technique used to measure magnetic fields generated by the small intracellular electrical currents in neurons) suggest that imagined movements are similar to imagined speech in that an internal forward model generates a somatosensory prediction produced during motor output planning. BCI software under development uses time-, frequency- and time-frequency-domain features of EEG signals to drive navigation and other behaviors in a 3D virtual environment and to drive a tube resonance model for speech synthesis. The evolution of this research beyond the MURI could lead to direct mental control of engineered systems by thought alone ranging from automobiles through construction equipment to computers.

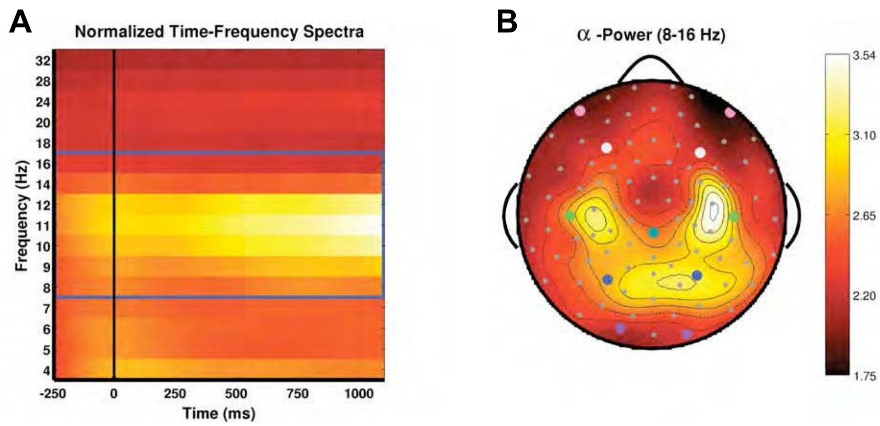


FIGURE 4

Covert spatial attention engages multimodal parietal areas as well as premotor and frontal areas. (A) Alpha-band power increases just prior to the 500 msec mark at which stimuli to be attended first appear. Increased power extends through 1,100 msec, the latest time at which stimuli to be attended appear. (B) The topographic distribution of alpha power, averaged across time, displays the parietal and fronto-central components characteristic of attentional networks revealed by functional magnetic resonance imaging (fMRI) studies of visual attention.

3. Dynamic Models of the Effect of Culture on Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Michele Gelfand at the University of Maryland, College Park. The objective of this MURI is to understand the effects of culture on collaborative and negotiation processes. Cross-cultural collaboration and negotiation are increasingly becoming an essential element of military combat and humanitarian operations (see FIGURE 5).

FIGURE 5

Inter-cultural negotiations. Understanding and applying culturally-appropriate interactions and negotiation tactics will significantly impact the success of these processes.

The goal of the MURI is to carry out a systematic examination of culture and negotiation and collaboration, with a particular focus on the Middle East. The first objective of the project is to develop a comprehensive understanding of core cultural values, norms, and attitudes within the Middle East. The second objective is to examine dynamic effects of culture on psychological and social processes in negotiation. The third objective is to examine dynamic effects of culture on collaboration processes, and the final objective is to examine how dynamical modeling and agent based modeling can help understand culture and negotiations and collaborations. The MURI initiated numerous efforts that span multiple methodologies (qualitative, experimental, survey, archival, computational) within each of these objectives.

4. Exploring Signaling Network Interactions Controlling Mouse and Salamander Limb Regeneration. This MURI began in FY09 and was awarded to a team led by Professor Ken Muneoka at Tulane University. The objective of this research is to identify and characterize signaling network interactions that control mouse and salamander limb regeneration.

The ultimate goal of this MURI is to establish the molecular-genetic foundation necessary for limb regeneration. The Mexican salamander is being used as a model organism (see FIGURE 6). The investigators are using a comprehensive approach to document all gene transcripts that are modified during limb regeneration in this model organism. The researchers will use this data to develop a complete regeneration specific microarray chip that can be used to gather data from mathematical modeling of temporal changes in cellular transcriptomes associated with regeneration, in particular, the reprogramming of fibroblasts. The team will model regeneration in the mouse digit tip that is mediated by blastema formation. The modeling is expected to identify specific nodes during the injury response that control whether a wound heals via scar tissue or via reprogramming to form a blastema and eventually regeneration. In the long term, the results of this research could potentially be used to initiate regenerative therapeutics to be tested on amputated limbs in a rodent model.

FIGURE 6

The axolotyl (Mexican salamander). This organism is capable of regenerating most of its body parts, and is being used as a model system for regeneration studies.

5. Mechanisms of Bacterial Spore Germination. This MURI began in FY09 and was awarded to a team led by Professor Peter Setlow at the University of Connecticut Health Science Center. The objective of this research is to decipher the biological mechanisms that underlie heterogeneity of bacterial spore germination with an emphasis on the slow germinating population

Most bacterial spores readily and quickly germinate after being exposed to appropriate growth conditions, a small percentage do not. Within the population, individual spores may germinate days, weeks, or even months, with serious implications. In food processing, the presence of slowly germinating spores results in a need for harsh processing conditions, such as high pressure and temperature, leading to a loss of food quality and appeal. Medically, delayed germination can result in disease appearance after antibiotic therapy has been discontinued. This research team is using a combination of "wet lab" experiments and computational modeling to understand the fundamental mechanisms of spore germination. This research may ultimately lead to strategies for preventing bacterial spore germination that could be used in food processing and medically-relevant therapeutic technologies, and for the enhancement of spore germination to be used in new methods of biofuel production.

6. Modeling Cultural Factors in Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Katia Sycara at the Carnegie Melon University. The objective of this MURI is to understand how cultural values, such as the highly-prized "sacred values," can shape the collaboration and negotiation process.

The team has already made interesting discoveries in these studies, including the observation of certain values called "sacred values" that are considered as essential to the identity of a given social group, thereby leading members of the group to respond defensively when these values are seen to be challenged or threatened (discussed further in Section III-H). One example of sacred values includes the observation that the Iranian nuclear program is treated as sacred by some Iranians, leading to a greater disapproval of deals that involve monetary incentives. In addition the team is exploring how humiliation may contribute to regulating relationships within Muslim countries. Humiliation seems to result in clashing behavioral tendencies that offer no regulatory strategies. Participants in the study motivated to change the status quo underestimated the extent to which the out-group moralized the domains of harm, care, fairness and justice. Further, participants motivated to maintain the status quo accurately identified that the out-group moralized harm, care, fairness and justice to the same extent that they themselves did. The investigators will replicate these studies in India and Israel/Palestine in the coming year.

7. Blast Induced Thresholds for Neuronal Networks. This MURI began in FY10 and was awarded to a team led by Professor David Meaney at the University of Pennsylvania. This research is jointly managed with the ARO Mechanical Sciences Division. The objective of this MURI is to understand the effects of a primary blast wave and how it can cause persistent damage to the nervous system and the brain at the meso- and micro-scale.

The research team will build and validate a model of the human brain/skull subject to blast loading and use this model to scale blast field conditions into cell culture and animal models. The project will develop multiscale blast thresholds for alteration of synapses, neuronal connectivity, and neural circuits (*in vitro* and *in vivo*) and will examine if these thresholds change for tissue and/or circuits in the blast penumbra. Finally, the researchers will determine the blast conditions necessary to cause persisting change in neural circuitry components (up to two weeks) and will correlate alterations in circuits to neurobehavioral changes following blast. This research should provide a basis for shifting defensive armor design efforts from defeating the threat based on material deformation, damage, and rupture, to mitigating the effects based on biological relevance. In addition the research may lead to medical applications for treating neurotrauma and in regenerative medicine.

8. Prokaryotic Genomic Instability. This MURI began in FY10 and was awarded to a team led by Professor Pat Foster at Indiana University. The objective of this research is to identify and extract the mathematical signatures of prokaryotic activity in DNA.

The investigators are characterizing fundamental parameters in the microbial mutation process in a superior model system, including both cell-mechanistic and evolutionary components. The research is a comprehensive effort with strong experimental and computational components. The team will determine the contribution of DNA repair pathways, cellular stress, and growth conditions on the mutation rate and mutational spectrum of *E. coli* using whole genome sequencing over the course of strain evolution. The team is extending this analysis to a panel of twenty additional eubacterial species. To understand the forces that define short-term and long-term evolutionary mutation patterns, a new class of population-genetic models will also be developed. The investigators will include mutant strains with known deficiencies in genome maintenance. Parallel analyses in such strains will produce larger data sets that define, by comparison to wild type strains, the contribution of each repair pathway to the overall mutational spectrum. Mutational changes characteristic to specific environmental conditions/stresses/genotoxicants can be analyzed in the context of the mutational signatures of individual repair pathway throughout the genome. Overall, the proposed research presents an unprecedented opportunity to uncover patterns of mutational variation among prokaryotes. The approach is unique in that the investigators are using a comprehensive whole-genome, systems-biology approach to characterize and understand DNA instability at a whole-genome level, across a comprehensive range of prokaryotes.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Development of Fieldable Brain Trauma Analyzer System. A Phase II SBIR contract led by Engineering Acoustics, Inc. is attempting to develop a system for the rapid analysis of mild traumatic brain injury (mTBI) suitable for near front-line use. The previous Phase I (and Option) effort provided a solid basis for the ongoing development of the device and protocol. The investigators refined the mTBI vibrotactile sensory acuity

assessment device and established the technical and clinical framework for expanded multi-site, clinical verification using the sports concussion model. The success of vibro-tactile illusion detection in evaluating intracortical signaling integrity shows that the fundamental structure of intracortical columns related to sensory calculation appears to be sensitive to concussions, and thus by extension to other mTBI. The objective of this Phase II effort is to expand the clinical verification of this system with a multi-site recruitment pool, and adds multisensory modalities (audio-visual) to the existing test to provide a more robust and sensitive test protocol without significant increase in complexity. This system is envisioned to package the needed expertise into an automated low power system that would permit very rapid determination of return to duty decisions, avoiding needless delays for medical evacuation, and thus helping to sustain the future fighting force.

2. Multisensory Navigation and Communications System. Two Phase I SBIR contracts were awarded to Engineering Acoustics, Inc. and AnthroTronix, Inc. with the goal of designing and building a proof-of-concept system that enables investigation of multisensory navigation and communications among dismount Soldiers. This system would enable dismount Soldiers to quickly navigate to or away from specified waypoints or areas, while maintaining radio silence and light security. The system should utilize real-time visual and tactile cues to enable hands-free navigation and critical communications when silence must be maintained. In addition, the system will log user actions and present queries to enable detailed and automatic assessment of performance accuracy, time, and situation awareness. A unique aspect of this system is its contribution as a research platform to investigate effectiveness of alternative tactile patterns and multisensory arrays. Flexible multisensory cues and data-logging capabilities will enable in-depth research in multisensory perception and decision making. The research will enable dismounted Soldiers to navigate to or away from specified waypoints or areas while maintaining radio silence and light security, which is directly responsive to future Army needs in tactical maneuver and land navigation under combat conditions. The research is directly responsive to future Army needs for alternative communication and navigation support methods for use in operational scenarios in which standard communication is not possible or desirable, as well as the need for instantaneous and simultaneous communication of relevant information to multiple team members, up and down the chain of command. This technology also addresses the need for unobtrusive and intuitive means for communicating with team members and for controlling unmanned assets. Haptic feedback displays, if integrated with GPS, enable Soldiers to navigate in low visibility conditions, hands-free (allowing the Soldier to hold his/her weapon) and eyes-free (allowing focused attention to surroundings as opposed to a visual display).

3. Energetics of Cognitive Performance: Regulation of Neuronal Adenosine Triphosphate (ATP). Two Phase I SBIR contracts were awarded to Gencia Corp. and Luna Corp. with the goal of optimizing neuronal ATP production capacity. Highly qualified and very experienced Soldiers routinely leave the Army because they are old. Since human performance capabilities decrease with increasing age, persons 42 years of age and older are ineligible to join the Army. There are many possible causes of reduction in physical and cognitive capabilities, including injury and disease, however a major factor is the aging of mitochondria. Mitochondria are the organelles that produce energy that powers human beings, and are essentially the “batteries” that power the Soldier. Given that ATP is the key energy storage molecule in the body, the ability to stimulate mitochondrial ATP production would extend the time that Soldiers remain fit for duty, boost Soldier physical and cognitive performance capabilities, and expand the age range of suitable recruits. The objective of this projects is to design, construct, and demonstrate proof of concept function for a high throughput assay to screen for compounds that increase adenosine triphosphate production in neurons. The libraries of compounds identified in these efforts may be tested in subsequent (Phase II) contracts.

4. Rapid, High Resolution Protein Separation System. A Phase II Chemical and Biological Defense (CBD) SBIR contract, led by Physical Optics Inc., is attempting to produce a high resolution system whereby proteins present in a complex mixture can be rapidly and reproducibly separated. The ability to obtain rapid and sharp separation of proteins from complex mixtures is an essential tool for biological research and has many potential applications in medical diagnostics and screening. This project aims to develop a laboratory prototype capable of separating a mixture of 20-30 proteins that vary in size and charge by as little as 3 Kd and 0.1 pI units within 15 minutes. Such a system could be optimized to allow qualitative and quantitative screening of specific biological markers that might appear after injury, such as protein markers produced in response to traumatic brain injury.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Targeting Neuronal Adenosine Triphosphate Production Capabilities for Optimal Performance. A Phase II STTR contract led by Eon Corporation is attempting to identify compounds that increase mitochondrial function, either through an increase in basal mitochondrial efficiency or an increase in mitochondrial copy number per cell. Mitochondrial performance capacity directly limits physical and mental performance capacity in humans and is a major driver towards reduced performance capabilities as humans age. The ability to stimulate mitochondrial biogenesis or oxidative phosphorylation, when needed, is expected to have a significant impact on Soldier performance capabilities and may extend the age limit for Army recruitment. The investigators will design and completely test a proof of concept assay for compounds that increase oxygen consumption through increasing mitochondrial copy number or by increasing the respiratory rate. They will validate the mitchondrial oxygen consumption metric with adenosine triphosphate synthesis and will determine the statistical variability of slopes and precision necessary to discriminate false positives and negatives. They will screen four libraries of compounds and will establish a methodology of prioritization for follow-up of mitochondrially active compounds.

2. Innovative Technologies for Effectively Treating Multi-drug Resistant Bacteria. A Phase II STTR contract led by PolyMedix, Inc., is attempting to develop a therapeutic that is effective against multi-drug resistant and biofilm-embedded bacteria. Widespread uses of antibiotics and bacterial adaptation have combined to make antibiotic resistant pathogens prevalent. Especially troublesome are bacterial strains such as methicillin resistant *Staphylococcus aureus* (MRSA), which are resistant to multiple antibiotics and extremely difficult to eradicate. Another agent of special concern is *Acinetobacter baumannii*, a bacterial agent that has natural resistance to multiple antibiotics and frequently infects wounds suffered by warfighters in Iraq and Afghanistan. To complicate the problem further, bacteria can form biofilms during infection of a host; biofilms often develop and persist on medical implants. Once embedded in biofilms, bacteria that are normally sensitive to an antibiotic are protected and will be resistant to antibiotic concentrations several orders of magnitude higher than normally lethal levels. Novel non-conventional antibiotics, such as those being developed by this STTR, that are effective against multi-drug resistant and biofilm-embedded bacterial strains will have an enormous impact on Soldier and civilian health.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Investigating Impact of Visual Fatigue. The objective of this HBCU project, led by Professor Celestine Ntuen at North Carolina A&T State University, is to establish a new capability in neuroscience, initiated with an 18 month project examining visual fatigue during the use of stereoscopic displays, including head-mounted displays (HMDs). The project will analyze physiological signals presumed to correlate with different workload conditions in order to uncover the onset of eye strain (fatigue) and its impact on task performance while using stereovision displays. The signals to be analyzed include alpha, beta, and theta band recording from EEG recordings. Various neuroimaging techniques, such as EEG and functional near-infrared imaging (fNIR; a spectroscopic method used to measure metabolic activity of neurons), will be used with physiological/behavioral measures, such as electroculography (EOG; a technique for measuring eye movements), to evaluate the changes in performance with fatigue while using stereo-HMD analogs. The Army relevance is of two types for this research - first, the establishment of a new laboratory that will actively use fNIR along with other more standard electrophysiological and psychophysical measures to examine human performance, and second, the project itself, which will examine the costs of HMD use in Soldiers with techniques that are portable and potentially fieldable. Data obtained can act to inform design and usage guidelines for HMD deployment in the field.

2. Elucidating the Mechanism of Phase Resetting in the Circadian Central Oscillator of Cyanobacteria. The objective of this HBCU project, led by Professor Andy LiWang at the University of California - Merced, is to elucidate the structural and biochemical basis of phase resetting in the cyanobacterial central oscillator.

The cyanobacterial central oscillator is composed of only three proteins: KaiA, KaiB, and KaiC. KaiA binds to and promotes the phosphorylation of KaiC, whereas KaiB hinders KaiA, allowing KaiC to dephosphorylate. These rhythmic interactions generate a ~24 hr oscillation of KaiC phosphorylation that produces circadian behavior in cyanobacteria. The investigator will develop a model of KaiA dynamics, determine how an oxidized form of a quinine analog shifts the dynamic equilibrium of KaiA, and will determine how oxidized DBMIB-induced perturbations to the dynamic equilibrium of KaiA shifts the phase of the central oscillator. Circadian clocks have strong effects on alertness and cognitive and physical performance and the rapid deployment of Army personnel across time zones has detrimental effects on human performance. If successful this research will provide the first insights into the structural and biochemical basis of circadian clock resetting for any organism. Understanding the biochemical basis of circadian clock resetting is necessary in order to develop effective neutralizing strategies for jet lag.

3. Investigating Inactivation of *Bacillus Anthracis* Spores Using Carbon Nanotubes. The objective of this HBCU project, led by Professor Liju Yang at North Carolina Central University, is to explore the potential of single-walled carbon nanotubes to inactivate *Bacillus Anthracis* spores, either alone or in combination with chemical treatment or near-IR irradiation.

Single-walled carbon nanotubes possess antimicrobial activities against bacterial cells, likely by puncturing the cell wall via their needle-like structure. This research will test whether the needle-like nanotubes can also damage the protein coat of bacterial spores and if this damage effectively inactivates the spores. Carbon nanotubes with various surface groups (-OH, -COOH, $-NH_2$) and of different lengths will be mixed with spores from a non-virulent Sterne strain of *B. anthracis*. Following treatment, the spores will be germinated and compared to untreated controls to determine the efficiency of spore inactivation. In addition the potential for enhanced spore inactivation will be explored through combination of treatment with carbon nanotubes and near-infrared radiation or chemical agents. These experiments will test the investigator's hypothesis that damage to the spore coat induced by the nanotubes will make the spores more susceptible to heating from near-infrared radiation or to damage by chemical agents. If the investigators are able to identify conditions at which carbon nanotubes effectively inactivate *B. anthracis* spores, the results may lead to new methods for decontamination of endospore-forming pathogens.

4. Investigating the Mechanism of UV-Induced Collagen Damage. The objective of this HBCU project, led by Professor Julian Menter at the Morehouse School of Medicine, is to determine how UV-induced collagen damage varies as a function of UV wavelength and atmospheric temperature.

The protein collagen, which comprises ~70% of mammalian skin, contains fluorescent moieties that are unstable to solar radiation. Previous studies performed by the investigator indicate that the photochemical fading of these fluorescent moieties caused by solar UV radiation may impact the structure of the collagen triple helix and therefore could result in significant connective tissue damage or provide a milieu favorable for skin cancer. This research will investigate how the wavelength of UV radiation and the atmospheric temperature impact collagen damage. The kinetics and temperature dependence of photochemical fading and fluorescence emission of purified mouse collagen will be determined both in the presence and absence of hyaluronic acid. The addition of hyaluronic acid more closely approximates the *in vivo* dermal matrix. The investigators will also determine if reactive oxygen species contribute to the direct chemical photoreactions that lead to collagen fluorescence fading. Collagen will be exposed to UV radiation in the presence and absence of molecular oxygen and a panel of reactive oxygen species will be measured (superoxide, hydrogen peroxide, hydroxyl radical, singlet oxygen) to determine their relative importance to UV-induced collagen damage. These experiments will also test the possibility that UV-irradiated collagen itself might generate reactive oxygen species that could lead to collagen degradation. These studies will provide a scientific basis for predicting the extent of deleterious reactions that might occur in deployed Soldiers as a function of UV exposure and atmospheric temperature. Also by establishing which UV wavelengths are most responsible for collagen damage, these studies may inform the design of sunscreens that more effectively protect against solar-induced collagen damage.

5. Characterizing a Novel Naphthalene Metabolic Pathway in *Rhodococcus Opacus*. The objective of this HBCU project, led by Professor Ashvini Chauhan at Florida A&M University, is to characterize a novel metabolic pathway discovered in a bacterial strain isolated from fuel oil contaminated soil.

Napthalene is a toxic contaminant commonly found in fuel as a byproduct of the petroleum refining process. Little is known of bacterial naphthalene degradation by organisms other than *Pseudomonas putida*. Preliminary data suggests that *Rhodococcus* is dominant in degrading naphthalene in soil but little is known about the metabolic pathways involved except that they differ from those in *Pseudomonas*. This study will provide an understanding of alternative pathways by which naphthalene is metabolized in the environment. More specifically this research will lead to a better understanding of the mechanisms by which Gram-positive soil bacteria adapt and mineralize xenobiotic compounds. Biochemical and genetic approaches will be used to characterize the naphthalene degradation pathway in this ubiquitous soil organism. Since naphthalene is a routine contaminant of fuel oil, diesel, and aviation fuel, it likely will be a contaminant at any site that dispensed these fuels, including virtually all DoD sites. Understanding how this contaminant is degraded by a novel metabolic pathway will help guide future environmental remediation efforts.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Investigating the Influence of Phosphorylation State on Cytoskeleton Filament Function. The objective of this PECASE, led by Professor Sanjay Kumar at the University of California, Berkeley, is to investigate the relationship between the phosphorylation state of unstructured protein domains in cytoskeletal filaments and the morphology and mechanics of the cellular cytoskeleton.

Cells converse with their physical environment through the cellular cytoskeleton, which is composed of an assembly of protein filaments. Unstructured protein domains surrounding these filaments drive the assembly of the cytoskeletal network by providing a steric barrier that repels adjacent filaments. These domains are often extensively phosphorylated, which may modulate the range and strength of the repulsive interactions between filaments. This research seeks to determine a quantitative understanding of the relationships between filament phosphorylation, repulsive forces and network architecture. In this project peptides with varying levels of phosphorylation will be attached to planar and spherical surfaces and probed by several microscopy techniques to measure the repulsive forces and conformation of the peptides relative to phosphorylation status. The phosphorylation state of filaments will also be modulated in cells and the effect on cellular mechanical properties and cell fate decisions will be assessed. If the relationship between filament phosphorylation and network assembly can be understood and controlled, it may enable cell form and physiology to be engineered by manipulating the phosphorylation state of cytoskeletal filaments. The results of this research could ultimately enable the design and development of smart materials with adaptive properties.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Life Sciences Division managed seven new DURIP projects totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to understand metagenomics, host-parasite interactions, and brain computer interfaces.

I. University Affiliated Research Center (UARC): Institute for Collaborative Biotechnologies (ICB)

The ICB is managed on behalf of the Army and is located at the University of California, Santa Barbara (UCSB), in partnership with the Massachusetts Institute of Technology (MIT), the California Institute of Technology (Caltech) and industry. The scientific objective of the ICB is to investigate the fundamental mechanisms underlying the high performance and efficiency of biological systems and to translate these principles to

engineered systems for Army needs. Through research and strategic collaborations and alliances with Army laboratories, Research, Development and Engineering Centers (RDECs), and industrial partners, the ICB provides the Army with a single conduit for developing, assessing and adapting new products and biotechnologies for revolutionary advances in the fields of biologically-inspired detection, materials synthesis, energy generation and storage, energy-dispersive materials, information processing, network analysis and neuroscience. ARO awarded the ICB $8.9 million in 6.1 funds for FY10, which was the second year of a $70 million contract that was renewed in FY09 for a five year period. In addition, $4.4 million was awarded this year for six 6.2 level projects including one new project.

In 2010, the ICB supported 59 faculty, 79 graduate students, and 41 postdoctoral fellows across 15 departments at UCSB, Caltech and MIT. The research falls into five Thrusts: (i) Biomolecular Sensors, (ii) Bio-Inspired Materials and Lightweight Portable Energy, (iii) Biotechnological Tools for Discovery (iv) Bio-Inspired Network Science, and (v) Cognitive Neuroscience. Detailed descriptions of each core research Thrust and corresponding projects are available at the ICB program website (http://www.icb.ucsb.edu/research). A U.S. Army Technical Assessment Board and Executive Steering Board annually review the ICB research portfolio, assessing the project goals and accomplishments, and set goals for the coming year.

J. DARPA Revolutionizing Prosthetics Program

The primary goal of this program is to develop the basic neuroscience and engineering needed to enable the realization of advanced prosthetic devices that function with the same motor capacity as the biological limb, including sufficient sensory feedback to the wearer. Research covers the entire field of human physiology and Soldier survival following trauma. The ARO Life Sciences and Materials Science Divisions currently co-manage projects within this program aimed at optimizing the programming and hardware for an upper limb prosthetic for home use as well as projects examining the detection of traumatic brain injury that could complicate prosthetic integration, laser treatment of intracranial hemorrhage, and the use of muscle signals in addition to brain signals for better prosthetic control, among others. The results of this research may ultimately provide full anatomic and functional restoration from injuries to enable injured Soldiers (or civilians) to return to duty.

K. IARPA Computational Cognitive Neuroscience Program

The goal of this program is to establish computational equivalents of the intuitive and insightful thought processes of human information analysts, with the long-term goal of enabling efficient preprocessing of the flood of data available in today's information ecology. The ARO Life Sciences Division currently co-manages projects within this program aimed at embodying common sense in tasks requiring the processing of visual and semantic geospatial data. If successful these projects will develop and test a form of artificial intelligence that can display the referential richness displayed by embodied and experienced (contextual) human cognition, with specific applications in the visual (object recognition) and verbal (semantic) domains, thus advancing the domain of computational neuroscience in uniquely human-usable ways.

L. JIEDDO Rapid Development of Counter-IED Capabilities Program

The goal of this program is to establish new approaches and capabilities for countering IEDs, from initial detection to mitigation of the effects following detonation. The ARO Life Sciences Division is co-managing several programs that range from pre-deployment psychological preparation to the development of experimental models of post-traumatic stress disorder, to research for updating physiological diagnostics and interventions following injury by IEDs, including minimal traumatic brain injuries.

M. DARPA Seven Day Program

In recent years global surveillance networks have determined that the frequency and diversity with which new infectious microorganisms are emerging is increasing. While these increases are in part due to better reporting, there are multiple examples demonstrating this increase is promulgated by changes in natural systems and

potentially the activities of humans. Examples of factors implicated in the increase in new, emerging and re-emerging pathogens include: increased animal-human interface; increased population densities and co-location of vulnerable species with pathogen reservoirs; climate change, particularly affecting migration and spread of vectors; and narrowing of genetic diversity among food animal stocks. The expansion of biomedical technologies on the global stage is also suspected to increase the risk of orthogonal and highly diverse microorganisms. One growing concern is the potential risk posed by the proliferation of genetic engineering technologies that can be easily redirected from beneficial to offensive purposes or for covert biological industrial sabotage of food animals. Together, these natural occurring and synthetic threat agents challenge current detection methods and could possibly defeat traditional medical countermeasures.

No group is at greater risk of exposure to new international pathogens, to bio-sabotage of food supply lines, or to attack from biological threat agents, than the U.S. Military. The traditional medical response for responding to large scale infectious disease outbreaks is to (i) quarantine exposed personnel (hours to weeks), (ii) identify and characterize the agent (usually within 0-90 days), (iii) develop a vaccine or therapeutic (1-14 years), and (iv) stockpile, distribute, and administer treatment. In cases where the pathogen is unknown or difficult to characterize, victims are likely to succumb before an effective therapy or vaccine can be developed, distributed and administered. The objective of this program, co-managed by the Life Sciences Division and DARPA, is to develop highly innovative approaches to counter any known, unknown, naturally occurring or engineered pathogen. The goals are to investigate novel technologies to prevent infection, extend survival until a curative response is available, provide transient immunity, and increase the onset of adaptive immunity.

N. DARPA Enabling Stress Resistance Program

The goal of this program, co-managed by the Life Sciences Division and DARPA, is to create a comprehensive, quantitative description of the impact of stress on the brain. This effort seeks to leverage cutting-edge technologies and recent advances in molecular neurobiology, neuroimaging and molecular pathway modeling as applied to animal models of acute and chronic stress. The objective of the effort is a proactive approach to stress mitigation, starting with development of a comprehensive understanding of the complex effects of multiple stressors on the brain. The program has the ultimate goal of the development and implementation of cognitive, behavioral, and/or pharmacological interventions that will prevent the deleterious effects of stress on the brain. The investigators will pursue their objectives through the creation of research teams to thoroughly investigate the multiple physiological pathways and molecular mechanisms involved in the brain's response to acute and chronic stress as well as physical, social, cognitive and affective stressors.

O. DARPA Surviving Blood Loss Program

The Surviving Blood Loss program, co-managed by the Life Sciences Division and DARPA, is developing novel strategies to radically extend the time warfighters can survive critical blood loss on the battlefield before initiation of fluid and blood resuscitation. Achieving this goal may allow increased time, perhaps many hours or even days, for evacuation, triage, and initiation of supportive therapies. An interdisciplinary effort is under way to develop a comprehensive understanding of energy production, metabolism, and oxygen utilization, and to identify and control the protective mechanisms that preserve cellular function despite critically depressed oxygen delivery. The specific goals of the program include discovering mechanisms to control the metabolic state on demand, including the induction of a hibernation-like state, and the development of low-volume therapies that reduce tissue demand for O_2 and metabolites when full resuscitation is not available.

Significant progress has already been made toward achieving program goals, including the proof of principle of metabolic rate reduction in mammals using hydrogen sulfide and hormone induced resistance. Exposure to low levels of H_2S was shown to induce a "hibernation-like state" in mammals, which is highly protective against blood loss or low oxygen environments. The treatment is hypothesized to reduce cellular O_2 consumption by both reversibly inhibiting the mitochondrial enzyme cytochrome oxidase and by acting as an electron acceptor alternative for oxygen. Resistance to the effects of trauma and blood loss was demonstrated with a single dose of the female hormone 17β estradiol (E2). The mechanism of action is likely related to the induction of widespread adaptive mechanisms at the biochemical, cellular, and physiologic levels.

P. DARPA Deep Bleeder Acoustic Coagulation Program

The goal of the Deep Bleeder Acoustic Coagulation program, co-managed by the Life Sciences Division and DARPA, is to develop a portable, lightweight, noninvasive, automated system for the detection, localization, and coagulation of deep bleeders that is operable by minimally trained personnel in the combat environment. The Division manages the single phase II effort in this program, a $11.3 million award to Siemens. Progress to date includes development of Doppler-based automated bleed detection algorithms, modeling and testing of high intensity focused ultrasound delivery and dosing, and creation of unique materials to enable testing on a full sized leg surrogate.

Q. DARPA Wound Stasis Systems Program

This program, co-managed by the Life Sciences Division and DARPA, seeks a materials-based agent(s) and delivery system that provides hemostasis (*i.e.*, arrested bleeding) targeted to damaged tissue and wound control capable of treating compressible and non-compressible wounds regardless of geometry and location. Successful completion will result in a hand-held delivery system that addresses military needs for control of blood loss and improved wound outcome.

R. DARPA Restorative Injury Repair Program

The vision for the Restorative Injury Repair program, which is co-managed by the Life Sciences Division and DARPA, is to fully restore the function of complex tissue (*e.g.*, muscle, nerves, skin) after traumatic injury on the battlefield. These injuries include both kinetic (*e.g.*, penetrating wounds) as well as other destructive injuries (*e.g.*, chemical and thermal burns, musculoskeletal injuries, blast overpressure). The goal of the program is to replace the current concepts of “wound coverage” by fibrosis and scarring with true “wound healing” by regeneration of fully differentiated, functional tissue. The program will achieve its goals by developing a comprehensive understanding of the wound environment, including cellular elements, matrix, inflammatory mediators, growth factors, nutrients, substrate utilization, biofilms, and ultimately processes of morphogenesis leading to anatomic and functional restoration.

S. DARPA Physical Intelligence Program

The goal of this program, parts of which are co-managed by the Life Sciences Division and DARPA, is to establish the physical foundations of intelligence using a coordinated effort that includes theory, implementation, and analysis. The objective of the theory domain is to develop and validate a physical formalism that unifies and expands ideas from diverse domains such as evolution, thermodynamics, information, and computation. The objective of the implementation domain is to demonstrate the first human-engineered open thermodynamic systems that spontaneously evolve non-trivial "intelligent" behavior under thermodynamic pressure from their environment. The objective of the analysis domain is to design analytical tools to support the development of human-engineered physically intelligent systems and to understand physical intelligence in the natural world. The Division currently co-manages a project within this program that is developing a unified formalism of physical intelligence from two complementary theories, will validate these theories and demonstrate physical intelligence in engineered chemical and electronic prototypes, and will develop analytical methods to quantitatively assess the intelligence of the prototype systems. If successful, this program will provide the foundations to enable novel engineered systems that exhibit physical intelligence.

T. DARPA Fundamental Mechanics of Gliding Flight in Snakes Project

The objective of this project is to determine the fluid mechanics, musculoskeletal anatomy, and tissue mechanics required to produce gliding flight in snakes. The project is co-managed by the Life Sciences Division and DARPA. The project will achieve its goals using integrated experimental and computational modeling studies. Experimental investigations will utilize 1:1 scale snake models and a low speed water tunnel. To investigate the dynamics and control of snake gliding, detailed 3D kinematics will be determined using previously obtained videographic data and dynamical modeling will be used to reproduce the snake's body movements and overall

trajectory. The musculoskeletal anatomy and tissue mechanics important for snake gliding will be assessed by comparing preserved specimens of well-gliding vs. poor-gliding vs. non-gliding snakes. The flying snake under investigation in this project (*Chrysopelea paradisi*) is one species of very few that can move across all terrains (*i.e.*, air, water and land) with exceptional efficiency. Understanding the basic mechanisms behind the snake's flight ability may enable the future development of novel biologically-inspired reconfigurable unmanned vehicles that will be effective in air, water or land.

U. DARPA Phytoremediation of Atmospheric Methane Project

The Life Sciences Division currently co-manages a DARPA project in phytoremediation. Phytoremediation involves the treatment of environmental problems (*i.e.*, bioremediation) using plants to mitigate the problem without the need to remove the contaminant material and dispose of it elsewhere. This joint project is aimed at assessing whether transgenic plants expressing the bacterial genes for soluble methane monooxygenase can metabolize atmospheric methane to methanol. The project will achieve its goals by developing vectors for expression of the essential subunits of soluble methane monooxygenase genes in plant nuclear and plastid genomes, transforming these vectors into plants, and assessing methane monooxygenase gene expression using colorimetric oxidation and real-time polymerase chain reaction (RT-PCR) assays. The transformed plants will also be tested for methane oxidation directly using closed vessels and gas chromatographic analysis of headspace. Global warming will have a profound impact on future defense operations (*e.g.*, in the Arctic) and has the potential for large scale humanitarian disruption. Methane accounts for 20% of human-caused heat retention in the atmosphere. Therefore, an effective and inexpensive method to remove methane from the atmosphere would be a valuable tool with which to combat global warming.

V. DoD-funded Microbial Forensics Program

Bacteria adapt to changes in their environment by changing the complement of genes being expressed, and if necessary, by inducing mutational pathways to modify their genetic makeup. In either case, the resulting bacterial cells contain information about the organism's history. The Life Sciences Division has developed and is managing a microbial forensics program, in coordination with DTRA, DARPA, DHS, and other agencies. The goal of this program is to determine factors that are necessary and sufficient to predict how an organism was grown (*e.g.*, *in vitro* vs *in vivo*, growth media, environmental growth conditions), how it was processed, and where it may have originated. Additional efforts are directed at mathematical and computational methods to integrate the resulting data for future use in high-fidelity predictive capabilities. The capacity to determine the cultivation history of a bacterial sample and its genetic relatedness to known strains will directly address the Nation's forensics and national security needs.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Life Sciences Division.

A. Discovering Neurological Code of Brain Signals for Speech

Professor Gerwin Schalk, Wadsworth Center, Single Investigator Award

The objective of this project is to conduct non-medically oriented research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output, and potential mechanisms that could ultimately lead to non-invasive (*i.e.*, non-surgical) methods of communicating speech using thoughts (*i.e.*, through imagined, unspoken words). More specifically, this project aims to characterize the brainwaves responsible for spoken or imagined words as measured through electrocorticography (ECoG; practice of recording brain signals using electrodes placed directly on the brain's surface). Based on the ECoG results, if investigators can determine and decode imagined words based on this more invasive measurement method, the project will then measure and analyze brainwaves recorded through electroencephalography (EEG; non-invasive method of recording brain signals using electrodes placed on the scalp). This effort, in combination with a similarly-focused MURI award co-managed by the ARO Computing Sciences and Life Sciences Divisions, ultimately aims to discover the neurological/physiological "code" of brain-to-muscle signals for speech.

In FY10, the researchers successfully characterized correlates of the Electro-Corticogram (ECoG, signals recorded from the brain's surface) to different aspects of speech and also determined to which extent these correlates may be used as a basis for a brain-based communication system using imagined speech. Existing data show that ECoG holds substantial information about a variety of aspects of speech. They also suggest that classification of discrete words or their components will likely not scale to a large number of items and suggest that the best avenue for a reliable brain-based communication system will likely be based on continuous decoding of motor/perceptual parameters. Specifically research efforts in FY10 delineated the brain signal features associated with speech by investigating spatiotemporal dynamics of ECoG signals. This provided empirical guidance for selecting appropriate ECoG features for discrimination of different aspects of actual and imagined speech and also adds to current understanding of language processing. ECoG activity was used to determine the vowels and consonants in the subject's spoken or imagined speech (see FIGURE 7).

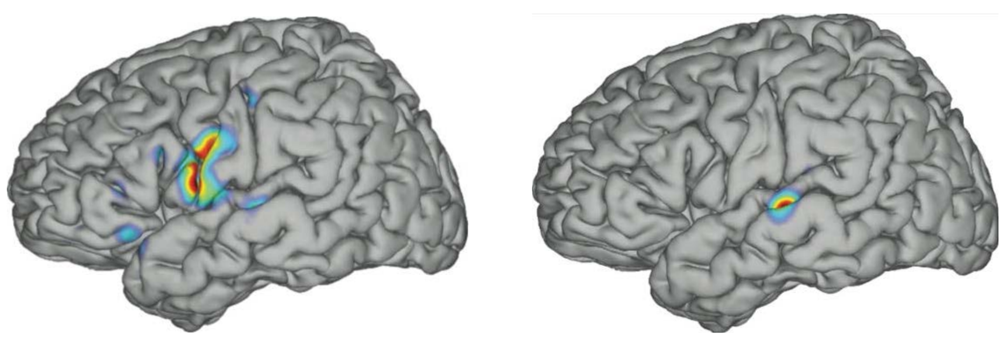


FIGURE 7

ECoG measurements may provide a map of imagined speech. These figures illustrate the brain areas that give information about the type of vowel (left) or consonant (right) in imagined speech.

These results, compiled in FY10, revealed that vowels and consonants in spoken or imagined words can be inferred using ECoG signals and also delineate the cortical areas that are most informative about the vowels and consonants. Further research delineated the temporal sequence of cortex participating in speech processing. The findings argue that cortical representation of speech is more of a networked and dynamic phenomenon in which information is encoded both in the cortical location but also in time. Additionally in FY10, the researchers determined the time course of ECoG gamma modulations during an overt and covert word repetition task. The results support a robustly networked model of speech with varied cortical participation of the perisylvian brain

sites contributing at all stages of language processing. Finally they identified whether the various stages and anatomic locations of speech processing could be differentiated by their spectral characteristics. The findings support the notion that separable frequency bands represent different neuronal populations participating in distinct aspects of speech tasks and thereby revise current understanding that suggested that high frequency signals are produced by one common physiological phenomenon.

In the long term, this research could ultimately lead to the eventual development of machine-mediated, direct able, verbal "telepathy." Future direct brain-to-military systems communications and control would provide a powerful advantage in speed and clarity when compared to channels that currently require actual transduction into sound transmitted via a medium (bone or air).

B. Studying Gene Networks Underlying Chronic Sleep Deprivation in Drosophila

Professor Ralph Greenspan, University of California, San Diego, Single Investigator Award

The goal of this project is to explore the effects of chronic sleep deprivation and identify the gene networks responsible for the sleep-deprivation response. In particular the team is working to identify genes whose expression is altered by sleep deprivation, thirst, and/or hunger. The investigator and his team discovered that 1,300 to 1,800 genes change in expression more than two-fold when the animal model system (*Drosophila melanogaster*; fruit fly) is exposed to these stress conditions. The team also discovered many interesting gene expression changes in response to hunger or hunger + thirst, including changes in the expression of (i) casein kinase I (CKI), a regulator of the circadian clock and influential in sleep regulation, (ii) TSG and BSK, members of the MAPKKK cascade, which together are involved in the epidermal growth factor receptor signaling pathway, (iii) SHAKER, a potassium channel gene implicated in sleep regulation, (iv) various genes involved in long-chain fatty acid synthesis, (v) cytochrome P450 genes involved in detoxification, (vi) various genes implicating additional signal transduction pathways in sleep response: AKT, the insulin-like receptor of the insulin signaling pathway (InR), PIP, a heparin sulfotransferase for HeS proteoglycans involved in growth factor signaling, and E(SPL), a complex of transcription genes involved in neuronal development, and (vii) two known stress-response genes, the heat-shock genes HSP60 and HSP70.

Based on these results, the investigators concluded that the impact of hunger and thirst on the expression of the epidermal growth factor receptor and the insulin-like peptide pathways reveals that the functions of these two disparate pathways are linked. In addition the team has also identified the cell types that secrete epidermal growth factor receptor ligands in the *Drosophila* brain, and found that those cells are the same cells that secrete insulin-like peptides. More importantly these cells are in the region of the brain that appears to be the fly's counterpart of the hypothalamus. The link between these two pathways is reinforced not only by conservation of the genes that determine the cell fate of neurons in the mammalian hypothalamus with those in the fly pars intercerebralis, but also because neurons in these regions share many of the same physiological functions in the adult, including sleep regulation, hunger response, and various other behaviors.

The investigators have also conducted preliminary behavioral tests of flies with mutations affecting either epidermal growth factor receptor signaling or insulin-like signaling. The research team discovered potent effects of either system on sleep as well as potent interactions between sleep and hunger. In the long term, these findings may enable the identification of specific genes that are affected in response to stressors and ultimately allow the identification of pathways that could be controlled through drug therapies.

C. Investigating the Mechanism of Reflective Camouflage

Professor Daniel Morse, University of California at Santa Barbara, Single Investigator Award

The objective of this research is to elucidate the biomolecular mechanisms underlying the dynamic reflective camouflage of squid. Squid of the *Loliginidae* family can reversibly actuate dynamic protein-based structures to control the color and reflectance of their skin. Reflectance is achieved within specialized cellular structures through modulation of the thickness and spacing of layers composed of reflectin protein. These protein layers have a high refractive index and are separated by layers of extracellular space with a low refractive index. This structure effectively acts a Bragg reflector, producing high intensity reflectance from the constructive interference of the reflectin protein layers. This research involves isolating and biochemically characterizing the reflectin proteins from the squid *Loligo pealeii* and identifying changes in protein conformation, association,

modification, and/or cofactor binding that lead to rapidly controllable changes in reflectance. Studies will then be performed at the molecular and subcellular levels to determine how changes to the reflectin proteins elicit reversible condensation and hierarchical assembly to form the Bragg reflector layers.

The investigator and his team have successfully cloned, expressed and purified the reflectin proteins and completed a comprehensive biochemical characterization. They discovered that upon induction of reflectance, the positive charge of the reflectin proteins is progressively neutralized by protein phosphorylation. This charge neutralization alters reflectin protein interaction and assembly within the reflective structures of the skin, which in turn alters the wavelength of light reflected, producing a change in the color of the reflective camouflage (see FIGURE 8). The investigators will explore how the condensation of the reflectin proteins changes the thickness, spacing and refractive index of the protein layers in the Bragg reflector structure.

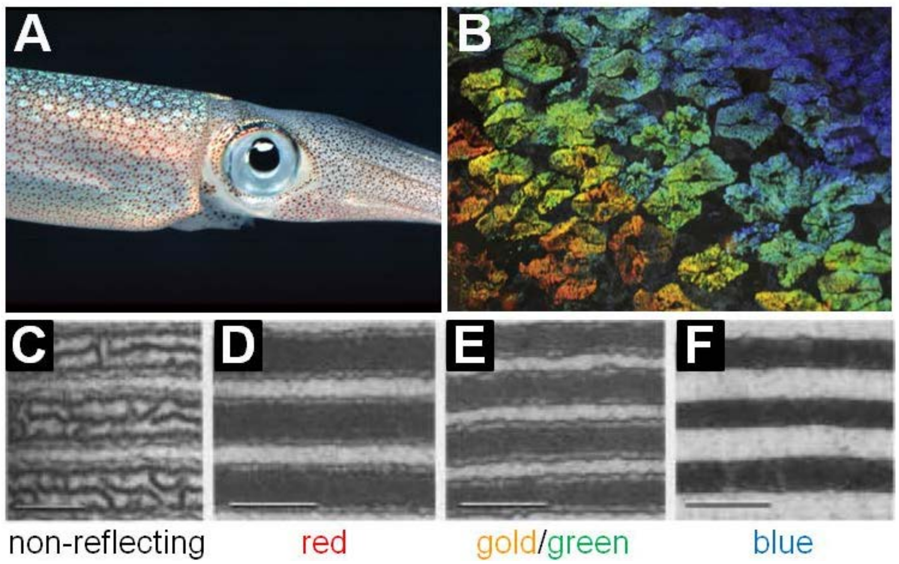


FIGURE 8

Reflective camouflage. (A) *Loligo pealeii* (squid) used as a model organism for these studies. (B) The reflective cells of *L. pealeii* can reflect light across the entire visible spectrum of color. (C) Positively charged reflectin protein layers are disordered and do not reflect light. (D-F) Upon activation of reflectance, the neutralization of protein charge allows condensation and assembly of the reflectin proteins into ordered reflective layers (dark bands). The thickness and spacing of the layers controls the color of reflectance.

Understanding how the squid controls its iridescent camouflage using reversible reflectin protein assembly may enable scientists to apply these unique biological mechanisms to the design of new materials, such as reflective camouflage or invisibility fabrics for the Army.

D. DNA Origami: Mechanisms for Breaking the Symmetry of Spherical Nanoparticles

Professor Hao Yan, Arizona State University, Single Investigator Award

The goal of this project is to design novel approaches for attaching multiple functional groups to spherical nanoparticles with control over the orientation of the groups relative to one another. Nanoparticles offer a unique platform in which to investigate the potential of controlled plasmonic interactions for future sensing systems. However it is extremely challenging to break the symmetry of a sphere and control the angles and distances between multiple functional groups on a nanoparticle. The proposed research calls for a creative approach in which the spherical nanoparticle is encased in a molecular cage formed by DNA origami. Functional groups can be attached to the outside of the DNA cage at precise locations to control their orientation in three-dimensional space relative to the nanoparticle within the cage as well as relative to other functional groups on the outside of the cage. This approach will also enable the generation of highly homogeneous populations of nanostructures for study. Direct attachment of functional groups to nanoparticles is difficult to control and often leads to highly heterogeneous populations. Measurements of these preparations therefore only represent the average effect of a

range of attachment sites. The introduction of the DNA cage will enable the preparation of pure populations of nanoparticles with precisely positioned functional groups for highly accurate measurements of plasmonic effects.

The investigators have successfully demonstrated the first known biological method for controlling the angles, distances, and orientations between symmetrical particles in three-dimensional space. The researchers constructed a non-spherical DNA cage and attached a gold nanoparticle within the cage, which effectively breaks the symmetry of the nanoparticles (see FIGURE 9A). They have also attached two gold nanoparticles to the outside of the cage at precise locations relative to the central particle and to each other (see FIGURE 9B).

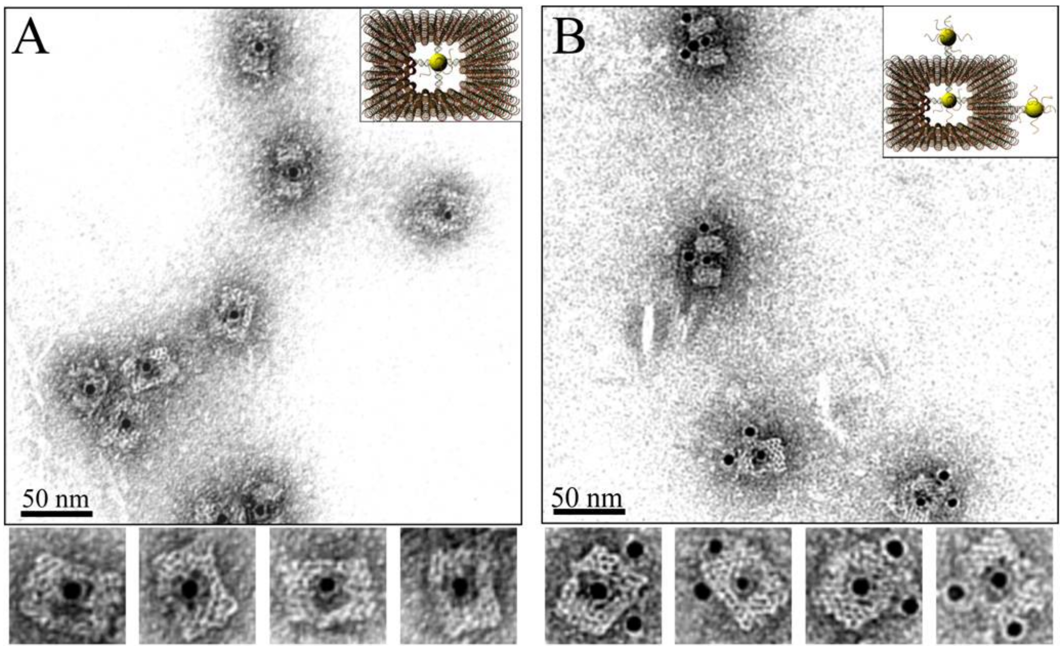


FIGURE 9

Breaking the symmetry of spherical nanoparticles. (A) 5 nanometer gold nanoparticles were attached to the interior of a DNA cage using four attachment points. (B) Two 5 nanometer gold nanoparticles were attached to the exterior of the cage using precise attachment sites. In both images, a schematic of the nanostructure is shown in the top right of the transmission electron micrograph and close-up images of individual nanostructures are shown below.

The angles and distances between different functional groups will be varied in three-dimensional space to investigate the impact of relative orientation on plasmonic effects. Future research also calls for investigations of arrays of multiple DNA cage/nanoparticle nanostructures. Control over the precise orientation of functional groups relative to metallic nanoparticles could allow unprecedented sensitivity in measuring plasmonic effects from nanoparticles and may be useful in single-molecule sensing applications. Moreover architectural control over structures at nanoscale dimensions may lead to opportunities in nanoscale multiplexing for a range of applications (*e.g.*, chem/bio detection, information encryption devices).

E. Inactivation of Spores of Bacillus Species by Wet Heat

Professor Yong-qing Li, East Carolina University, Single Investigator Award
Professor Peter Setlow, University of Connecticut Health Science Center, Single Investigator Award

The goal of these projects is to understand how bacterial spores are killed by wet heat (*i.e.*, heat transferred through liquid). Some bacteria, including those that cause food spoilage, anthrax, and botulism, take on a highly protective dormant structure called a spore. To understand how bacteria can be killed requires studies of germination, the process during which bacteria emerge from dormancy. While dormant spores are relatively hard to kill, resistance to inactivation by heat or other stressors such as disinfectants is lost upon germination. Consequently understanding the mechanism of spore germination could lead to ways to block germination, thus

preventing spores from causing food spoilage or disease. Alternatively stimulating spore germination would make it much easier to kill the spores and again prevent food spoilage and disease.

The investigators have successfully developed innovative technologies to study early stages of spore germination (see FIGURE 10). A classic method of observing spores is to use phase contrast microscopy. As light passes through the spore, a phase shift in the light occurs that make the spores appear bright against a black background (phase-bright). As the spores germinate, a small molecule calcium dipicolinic acid (CaDPA) is released and replaced with water; Raman spectroscopy can be used to assess the level of CaDPA in the spores. As the spores become fully hydrated, they lose refractility and become dark (phase-dark).

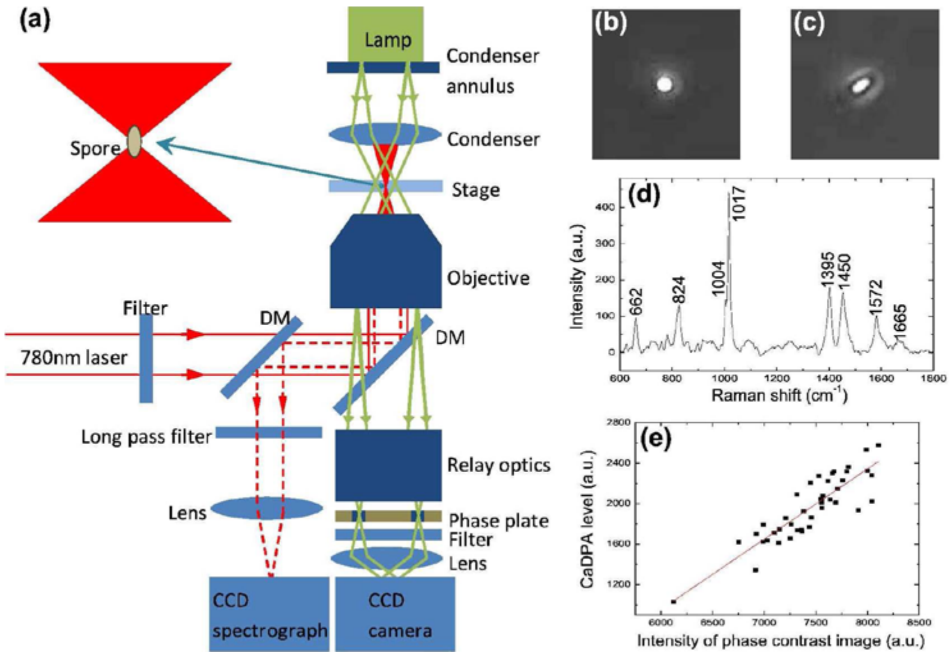


FIGURE 10

Experimental approach to examine bacterial spore killing. This approach utilizes phase contrast microscopy, Raman spectroscopy, and optical trapping. (A) As shown in the synthetic schema of the setup, the solid red is the optical trapping and Raman excitation beam, the dashed red is the backward Raman scattering light, and the solid green is the phase contrast imaging light; DM denotes a dichroic mirror. The phase contrast images are of (B) of a trapped dormant *B. cereus* spore and (C) the same spore in picture (B), recorded by temporarily blocking the trapping laser such that the spore re-aligned. (D) A typical Raman spectrum of a trapped dormant *B. cereus* spore is shown with band intensities expressed in arbitrary units (a.u.), with the CaDPA-specific band appearing at 1,017 cm^{-1}. (E) The intensities of the CaDPA-specific band versus the intensities of phase contrast image are shown for 42 trapped single dormant *B. cereus* spores; the red curve is a fitted line.

By combining phase contrast microscopy with Laser Tweezers-Raman spectroscopy, previously developed by the investigator, specific molecular changes occurring during germination of spores can be correlated with refractility. The researchers are using a highly efficient CCD and spectrograph and have increased the time resolution of Raman spectroscopy to allow a two-second scan, an increase of approximately ten-fold as compared to their previous work. Interestingly the team discovered that the phase contrast intensity of individual dormant spores was proportional to the CaDPA content of the spore. They also showed that the transition from phase-bright to phase-dark corresponded precisely with complete CaDPA release as shown with Raman spectroscopy. This direct correlation allows the change in refractility to be used as a surrogate for germination and enables simultaneous analyses of hundreds to thousands of individual spores.

Since the behavior of large numbers of individual microorganisms can be evaluated at the same time, this technique revealed differences in the behavior of genetically identical organisms. By using this newly developed technique, the researchers were able to pinpoint the likely phase in the spore germination process where variability is observed.

F. Vaccine Design Using MicroRNA-mediated Viral Attenuation

Professor Benjamin tenOever, Mt Sinai School of Medicine, PECASE Award

The objective of this research is to determine how host generated microRNA molecules interact with invading viruses. The investigator is testing the hypothesis that viruses can be attenuated by modifying the viral genome to be an exact complement to a microRNA expressed in the host tissue of interest.

Influenza A virus is a seasonal pathogen responsible for the deaths of over 50,000 people in the U.S., annually. In humans the viral life cycle begins when the virus enters lung bronchial epithelial cells (see FIGURE 11). The eight individual non-coding strands of RNA comprising the viral genome, migrate to the host cell nucleus where individual strands are transcribed by a viral RNA-dependent RNA polymerase. The transcripts are then transported to and translated in the cytoplasm. At a later point in time, the RNA-dependent RNA polymerase switches from viral genome transcription to replication. Newly synthesized genome segments are then packaged into viral capsids using the previously synthesized proteins.

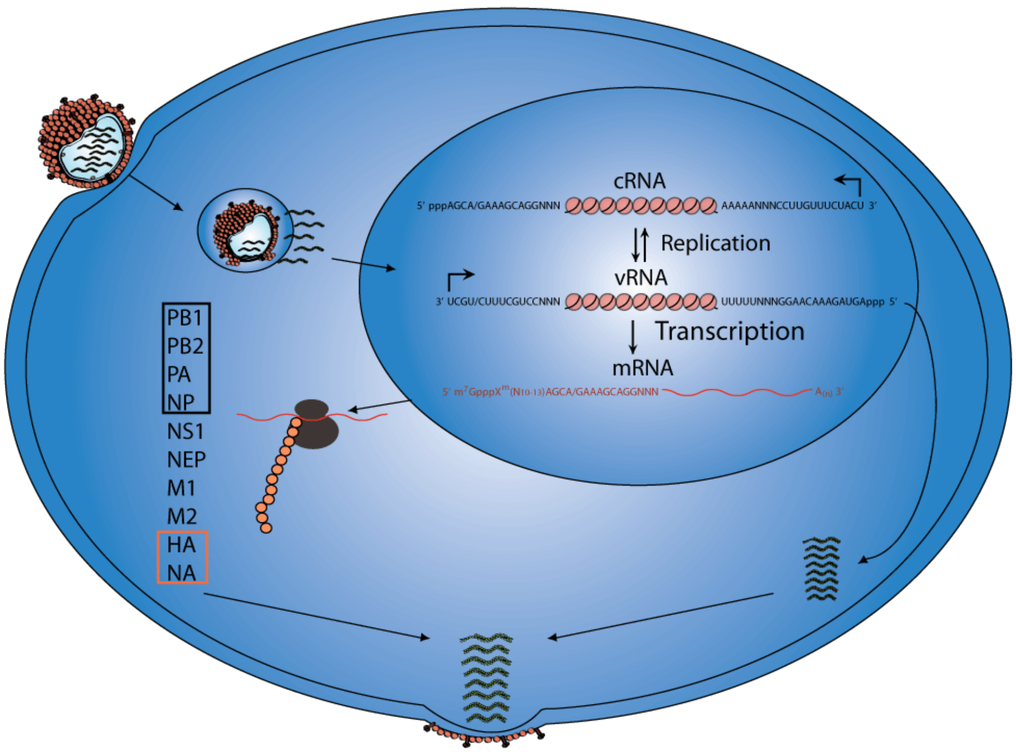


FIGURE 11

Influenza A life cycle. The virus is taken up by the cell and the 8 segments of the viral genome (vRNA) are transported to the nucleus. The vRNA is transcribed by a viral RNA-dependent RNA polymerase to produce messenger RNAs (mRNAs) which are transported out of the nucleus and translated to produce the 10 viral proteins (PB1, PB2, PA, NP, NS1, NEP, M1, M2, HA, and NA). Subsequently the RNA-dependent RNA polymerase switches from transcription to replication and synthesizes RNA strands (cRNA) that are complementary to the vRNA. vRNA strands synthesized from the cRNA templates migrate to the cytoplasm and are assembled with the previously synthesized proteins to form mature viral particles.

Live attenuated influenza A vaccine virus strains are developed annually due to the high rate of mutation and segment exchange. Attenuation is normally achieved by conferring temperature sensitivity upon the virus. These viruses are then grown to high titers in chicken eggs, purified, and mixed with other influenza strains to comprise the final influenza vaccine. The investigator has proposed developing a microRNA strategy for virus attenuation. MicroRNAs are known to be present and to influence RNA stability and translatability in a wide range of eukaryotic cells, often in a species- or tissue-specific manner.

The researcher and his team have successfully used deep sequencing to identify the sequence of microRNAs produced in human bronchial epithelial cells and in chicken allantoic membrane cells. MicroRNAs that were found to be highly produced in mouse and human bronchial epithelial cells but not in chicken allantoic

membrane cells were identified as potentially useful for virus attenuation. Highly conserved regions of the Influenza A virus genome were identified that were close matches for the reverse complement of the microRNAs. Although no perfect matches were found, several sites were identified that only required minor sequence modifications. Modifications to one or two virus protein coding sequences that caused the least disruption to the gene products (*i.e.*, the encoded amino acid was not changed, or a conservative amino acid was substituted) were introduced into the viral genome.

When inoculated into eggs, the modified viruses replicated and produced progeny at numbers similar to the unmodified virus. However when inoculated into the mouse model via inhalation, the modified viruses were attenuated by approximately three orders of magnitude, when compared to the unmodified virus, and elicited a robust immune response. These data establish the validity of species specific microRNA methods for rapidly developing new attenuated virus vaccine strains. The degree of virus attenuation can be modulated by varying the number of microRNA binding sites on the viral genome. Further since the mechanism of attenuation is different, strains produced by this method could be used in conjunction with temperature sensitive attenuated strains for added vaccine safety.

This newly developed attenuated virus vaccine production platform could be readily adapted to any of the negative strand RNA viruses, including Crimean-Congo Hemorrhagic Fever virus, Dengue Fever Virus, or West Nile Virus, and has the potential to be adapted to other classes of viral pathogens. Further studies of microRNA interactions with pathogens will provide unprecedented insight into how viral pathogens are able to usurp the host's cellular machinery while evading the host's defenses.

G. Anisotropic Nanostructured Materials for Electrochemical and Photovoltaic Energy Conversion

Professor Bradley Chmelka and Songi Han, University of California, Santa Barbara, ICB (UARC)

The objective of this research is to investigate novel inorganic-organic hybrid membranes with controllable orientation and to determine whether functional elements can be incorporated to yield previously unavailable properties of ion or electron conduction, photon absorption, and/or mass transport. A longer term scientific objective is to understand the variables influencing, and the ability to control, the interactions between functional components during materials synthesis and processing. If successful this research could ultimately allow the design of novel materials to meet energy-related needs of the Army with respect to energy generation, efficiency, storage, and management. This research will reveal the conditions for incorporating diverse functional molecular guest species into these hybrid membranes for targeted energy applications. In the longer term, by embedding the light-harvesting protein proteorhodopsin (PR; a transmembrane protein found in marine bacteria that uses sunlight to pump protons across the bacteria membrane) into a highly ordered silica membrane host (see FIGURE 12), the investigators may be able to harness the light-driven proton pump and create a cell that can harvest solar energy.

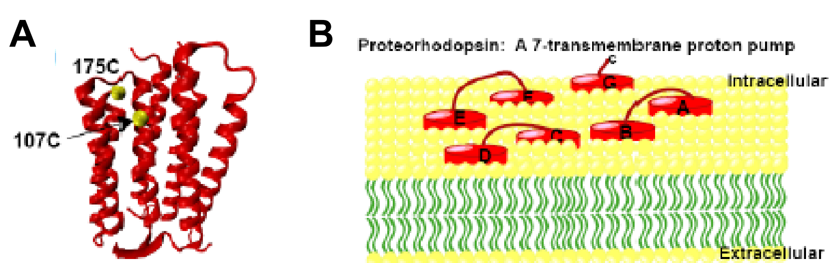


FIGURE 12

Schematic of proteorhodopsin-embedded membrane. Schematic diagrams of (A) the structure of a single proteorhodopsin (PR) molecule and (B) configuration of several PR molecules aligned across a cell membrane.

The research exploits a recent breakthrough by Professor Chmelka's group in controlling the processing conditions to prepare highly aligned cylindrical channels that can be oriented perpendicularly, longitudinally, or laterally with respect to a substrate in continuous or patterned films. Using this strategy, which relies on block copolymer-directed assembly, the researchers have successfully produced nanostructured silica and titania channels with controllable dimensions, orientational order across macroscopic (> cm) length scales, and a high

degree of hexagonal order (see FIGURE 13). A key advantage of this approach is the high degree of controllable ordering that allows for significantly enhanced transport of ions, electrons, and/or diffusing guest species.

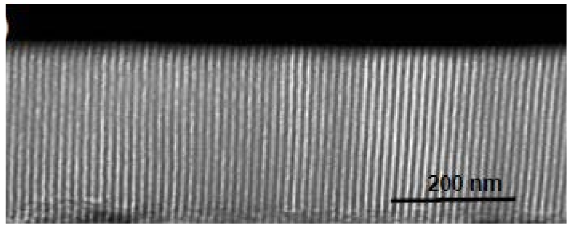


FIGURE 13

Highly ordered silica film. Cross-sectional focused-ion-beam transmission electron microscope image of a 600-nm-thick 1-cm^2 patterned film showing highly hexagonally ordered nanoporous silica with 8-nm cylindrical channels oriented vertically with respect to the substrate

Although the research is in the early stages, within just a six month period the researchers have successfully incorporated PR into vertically aligned silica membranes without significant loss of functionality. Retaining biochemical functionality (*e.g.*, proton pumping activity) in such a matrix presents a significant fundamental challenge. The researchers have made substantial progress in identifying the optimal solvent conditions that yield a high degree of desirable geometric and orientational order of the membranes, while being compatible with the guest PR species, overcoming challenges with previous formulations that irreversibly denatured the PR.

Through collaborations with Professor Han's group, the investigators have verified the alignment and intact functionality of PR in the silica nanochannels (see FIGURE 14). State-of-the-art techniques, including nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy were also used to elucidate local environmental effects on PR electrochemical and photophysical properties and guide further improvements in material processing.

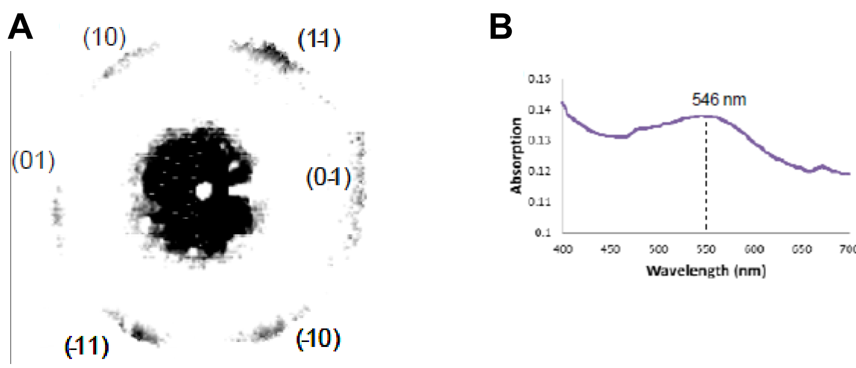


FIGURE 14

Measurements of membrane incorporating PR. (A) Small-angle X-ray scattering pattern of a hexagonal nanostructured silica-PR membrane, whose six-spot pattern indicates a high degree of orientational ordering of the nanochannels vertical to the substrate. (B) UV-Vis spectrum of the same film, showing a signal at 546 nm, characteristic of PR.

Given that the researchers have successfully demonstrated the feasibility of incorporating functional PR in aligned nanostructured silica host matrices, the team is now focusing efforts to increase PR loading, demonstrate and quantify their proton-transport properties, and eventually integrate the PR-containing nanostructured silica membranes into membrane-electrode assemblies. The materials, processing, functionalization, and characterization objectives are general in scope and are expected to provide understanding that can benefit applications and processes based on ion-conduction, photovoltaic, and electrocatalyst materials and devices. For example, proton-exchange membranes with aligned proteorhodopsin guest species are expected to provide novel combinations of high proton-conductivity, unique light-triggered response, film processability, robust mechanical stability, environmentally benign species, and compatible device integration properties. The underlying and unifying processing principles show promise for varied and broad applications, such as membranes for fuel cells, supercapacitors, electrodes, and photovoltaic energy generation.

H. Modeling Cultural Factors in Collaboration and Negotiation.
Professor Katia Sycara, Carnegie Mellon University, MURI Award

The objective of this project is to understand the role of culture in negotiation and collaborations. The process of negotiation involves actors (*i.e.*, participants) with varying perceptions, cultural values, and possible goals and objectives. Offers on the part of one party to another may yield unintended consequences that limit the chances for a desirable outcome. One possible impediment to effective negotiations concerns morally-motivated behavior in the form of "sacred values" that can create a backfire effect. Sacred values, which are values considered to be essential to the identity of a given social group, can lead an actor to be immune to classical cost/benefit considerations, instrumental motivations, and rational conceptions of success.

This study recently completed experiments with 720 Palestinians in the West Bank and Gaza Strip investigating the backfire effect (see FIGURE 15). The experiments compared the responses of moral absolutists to non-absolutists with respect to two conditions on a deal to settle the Israeli-Palestinian dispute. As shown in the figure, the two deals presented to the study population were designated as *Taboo* and *Taboo+*. The *Taboo* proposal called for a peace treaty between Israel and the Palestinians, with Palestinians recognizing the sacred and historic right of the Jewish people to Israel, and establishment of a Palestinian state in 99% of the West Bank and Gaza, while the *Taboo+* proposal included the same conditions with the addition of a monetary incentive, requiring Israel to pay Palestine $1 billion per year for ten years. The results revealed that although most responders reacted similarly to the *Taboo* proposal, a subset of responders (moral absolutists) responded in favor of violence when a monetary incentive was added (*Taboo+),* while the other subset (Non-absolutists) did not approve of violence (*i.e.*, favorable response). These results suggested that the Moral Absolutists subgroup considered the *Taboo* proposal to be a "sacred value" and were insulted when a monetary incentive was added (*Taboo+*), whereas the non-absolutists responded favorably to the monetary incentive.

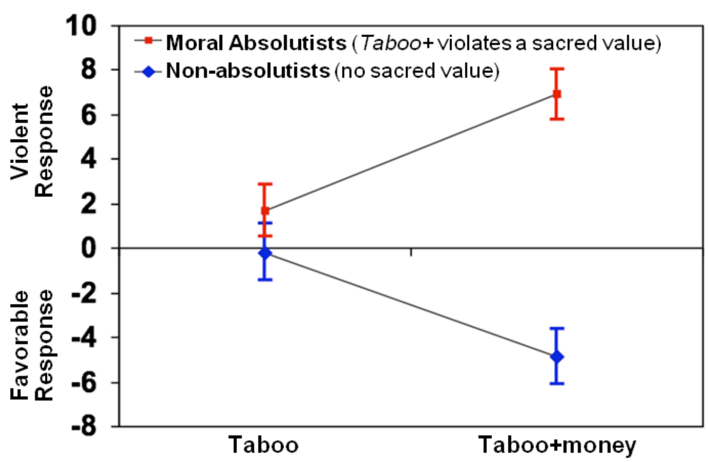


FIGURE 15

Adding monetary incentives to proposals involving sacred values can lead to a backfire effect. The plot displays results of surveys of 720 Palestinians in the West Bank and Gaza strip. The responders were given two potential deals (*Taboo* and *Taboo+*, described in the text), and their responses (y-axis) were found to be either neutral (0), violent (positive values), or against violence (negative values). The results suggest that the moral absolutists subgroup considered the *Taboo* proposal to be a "sacred value" and were insulted when a monetary incentive was added (*Taboo+*), whereas the non-absolutists responded favorable to the monetary incentive.

These findings provide important insights into the theoretical underpinnings of individual behavior in negotiation cultural settings and contexts. An understanding of the backfire effect provides a critically important framework for the conduct of more effective negotiations in cross-cultural settings, in which typical Western approaches may be counterproductive.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Apparatus and Method for Quantitative Assessment of Brain Function

Investigator: Engineering Acoustics, Inc., SBIR contract
Recipient: MRMC, Telemedicine and Advanced Technology Research Center (TATRC)

The goal of this research is to develop a portable device and testing protocol for the objective and quantitative diagnosis of acute minimal traumatic brain injury (mTBI) suspects. The condition of mTBI is hypothesized to involve derangement or damage to the underlying cortical network. In particular fundamental building blocks of the cortex in the brain are changed in such a way as to limit the functional connectivity within and between cortical columns. This project is developing a multimodal approach based on sensory illusions and configured as a test of neural connectivity. A portable, low cost diagnostic device that is able to quantitatively and objectively screen patients for brain injury, including mTBI and concussion, would have significant benefits to the military and civilian populations. The ability to objectively screen Soldiers who have been exposed to any head injury risk factors would be a significant advancement. Quick and accurate field screening of acute mTBI will lead to faster and better medical intervention and command decisions and reduce risk for post-concussion syndrome. This is of critical importance in the battlefield where potential operational risks posed by any possible cognitive and behavioral problems may be greatly reduced.

A patent was submitted for the apparatus (see FIGURE 16) and method for the quantitative assessment of brain function that was developed by an SBIR Phase 1 performer. The results were provided to MRMC-TATRC and contributed to the successful initiation of a Phase 2 SBIR contract that began this year (refer to Section II-D.1).

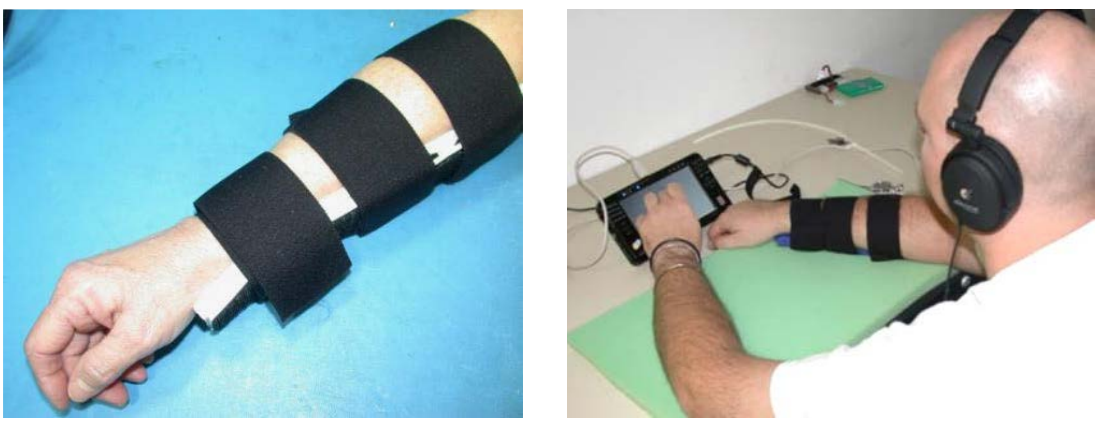


FIGURE 16

Apparatus for quantitative assessment of brain function. The vibrotactile array (left) is end positioned to coincide with the start of the trapezium (base of the thumb); (right) a volunteer is completing a vibrotactile mTBI assessment test.

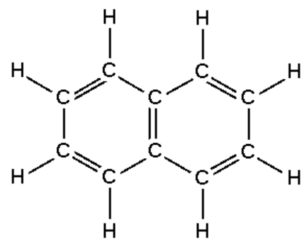
B. Naphthalene Dosimeter

Investigator: Photon Systems, Inc., SBIR contract
Recipients: DARPA; MRMC; National Institute for Occupational Safety and Health (NIOSH)

Naphthalene is a byproduct of the fuel refining process and is found in many fuels, including the fuel refined to the Jet Propellant 8 (JP-8) standard. Naphthalene is an aromatic compound that rapidly vaporizes (see FIGURE 17). This chemical has been identified as a serious health hazard for personnel working with JP-8 and other fuels containing naphthalene. A SBIR contract with Photon Systems, Inc., has been focused on designing and creating a dosimeter capable of accurately assessing naphthalene exposure levels. Regulatory

changes are expected that will require DoD personnel working with JP-8 to be able to monitor exposure in real time in order to be able to keep personnel exposures below NIOSH limits. In addition naphthalene exposure will enable human data to be obtained; the EPA decision to classify naphthalene as a likely carcinogen is based on rodent data. The shape of rodent noses and differences in the p450 pathway make it difficult to extract rodent data to humans and direct measurements on humans are necessary.

Other agencies, including DARPA, NSF, NIEHS, and NIOSH, have now invested in this research with the aim of expanding the range of measurable analytes within the dosimeter and they are actively working to validate the dosimeter via human testing. This SBIR project and the collaborating agencies are creating a dosimeter that will enable DoD to protect warfighters working with JP-8 and will enable the continued use of JP-8 containing fuels. Given that DoD uses 5.5 billion gallons of JP-8 each year, and exposure to JP-8 represents the single largest source of chemical exposure to DoD personnel, this investment will lead to improved Soldier protection.



Naphthalene
$C_{10}H_8$

FIGURE 17

Structure of naphthalene. JP-8 and other military-grade fuels contain naphthalene. A naphthalene dosimeter, for use in measuring levels of personnel exposure to the compound, is being developed by this SBIR contract. Based on the progress of this contract, DARPA, MRMC, NIOSH, and others are now actively working to validate the naphthalene dosimeter via human testing.

C. Structure-Informed Bioengineering of Theromostable *Pyrococcus Furiosus* Prolidase

Investigator: Professor Amy Grunden, North Carolina State University, Single Investigator Award
Recipient: Edgewood Chemical Biological Center (ECBC)

The objective of this project is to engineer a prolidase enzyme from a thermophilic bacterium and determine whether it can be used in the decontamination of nerve agents under field conditions. Prolidases are enzymes that normally catalyze the hydrolysis of the bond between an α-carboxyl group and proline or hydroxyproline. They are also active against the chemical warfare nerve agents sarin and soman, and have been proposed for use in detoxification of contaminated equipment and materiel. Using molecular biology and directed evolution techniques, the investigators have modified the enzyme so that it retains catalytic activity at 37°C whereas the original enzyme lost all activity at temperatures below 80°C. The modified enzyme is currently being evaluated for activity against nerve agent analogs at ECBC. Enzymes from thermophilic bacteria are extremely stable. The modified enzyme or derivatives from it will provide another weapon in the decontamination arsenal should chemical nerve agents ever be employed.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Actionable Variation in Human Genes

Professor Jasper Rine, University of California, Berkeley

The objective of this research is to identify single nucleotide variants in the human genome that result in suboptimal performance of individual enzymes, and to identify which of these variants can be rescued (*i.e.*, restored through intervention). In the next year, the investigators will examine nonsynonymous single nucleotide polymorphisms in five prototypical B6, niacin, riboflavin, and thiamine-dependent enzymes for functional impact and vitamin responsiveness. Variants will be tested for function and rescue-ability in the model eukaryotic organism *Saccharomyces cerevisaie* (*i.e.*, baker's yeast). The *in vivo* function of the proteins will be measured individually in a cell-based assay in which the human gene is expressed and functionally complements an *S. cerevisiae* cell that has had its own gene for the orthologous enzymes removed from the chromosome. Expression of the human gene is drive by a heterologous promoter and terminator so that the differences measured reflect differences intrinsic to the protein itself. The expression level of the human gene will be modulated so as to restore growth but remain limiting. Defined growth medium will be used to enable titration of the exogenous cofactor or to bypass the cofactor pathway entirely. Qualitative assessments of gene function will be made on solid medium while quantitative measurements of growth rate will be determined by measuring cell growth and division over time in a liquid culture. Based on these data, research in subsequent years will focus on determining the relative activities for each mutant protein and the activities and the vitamin responsiveness of each variant will be categorized.

In the long term this effort will help meet the Army and DoD goals of improving Soldier performance. This approach leverages NIH's investment in sequencing the human genome as well as recent advances in the biotechnology industry which have significantly lowered the cost of genome sequencing. The proposed research is the first step to using information on human genetic variation in a positive way to easily improve human health and performance.

B. Mechanics of the Adhesive Properties of Ivy Nanoparticles

Professor Mingjun Zhang, University of Tennessee

Adhesive mechanisms used by biological species represent exciting opportunities for biomimetic systems with unique capabilities. While some biological adhesive systems have been widely studied, including the gecko and the sea mussel, the physical properties that allow ivy to cling to and climb surfaces have been widely neglected. Charles Darwin reported that a single ivy adhesive disc weighing 0.5 milligram could support a weight of two pounds. Thus the force generated by the ivy adhesive disc is about 1.8 million times greater than its own weight, and the adhesive force of mature ivy may be even greater.

Professor Mingjun Zhang's research group at the University of Tennessee recently discovered that the adhesive secretion produced by ivy rootlets is composed of nanoparticles (see FIGURE 18). The ultimate goal of this project is to fully characterize the mechanical properties of ivy adhesive at both the microscopic and macroscopic levels and to relate the microscopic features of the adhesive to its macroscopic properties. The team is currently investigating the chemical composition of the nanoparticles. Preliminary research has suggested that the particles may contain a protein component. It is anticipated that the researchers will test for the presence of protein in the nanoparticle fraction of the adhesive, and if found, the sequence of the protein(s) will be determined. The team will also characterize the intra- and inter-molecular bonding forces between (i) nanoparticles in the ivy adhesive, (ii) the nanoparticles and the adhesive polymer matrix, and (iii) the nanoparticles and the affixing surface, using atomic force microscopy and nanoindentation.

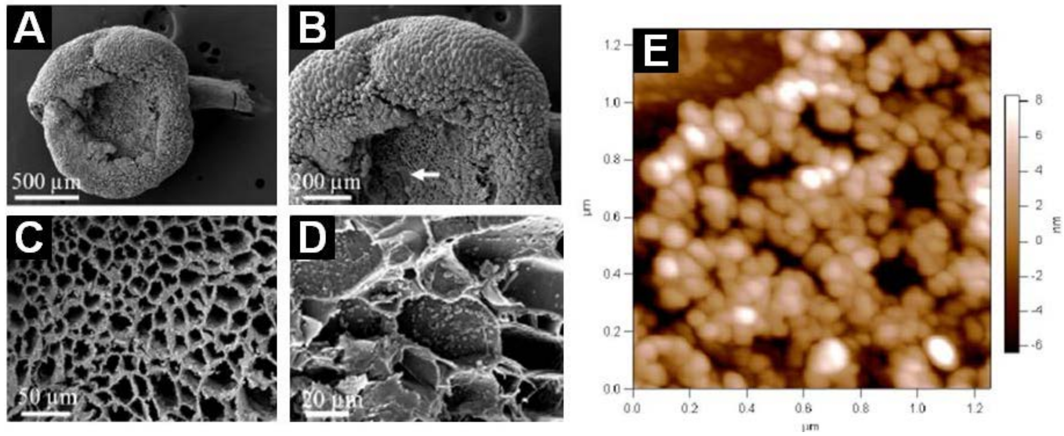


FIGURE 18

Ivy adhesive nanoparticles. The panels within the figure are (A-B) scanning electron micrographs of the adhesive disc of Boston ivy; images are facing the affixing surface of the disc, (C) micro-channels of the adhesive disc that secrete the nanoparticle adhesive, (D) a cross-section of the micro-channels showing nanoparticles within the channels, and (E) atomic force microscopy topographic image of ivy adhesive nanoparticles (image is 1.25x1.25 microns).

The elucidation of the chemical composition and the mechanical properties of ivy nanoparticles may enable future research in which the adhesive polymer matrix and/or the nanoparticles are altered to create new material properties. This research may also inspire biomimetic approaches for the design of new materials with superior surface adhesion for military applications.

C. Synthetic Biological Design of Photosynthesis

Professor Pamela Silver, Harvard Medical School

Photosynthetic organisms capture about 11% of incident light energy in the form of energized electrons. Normally these electrons are distributed throughout the metabolic pathways in an organism based on chemical equilibria. Ultimately much of this chemical energy is converted to carbohydrates by a series of efficient enzymatic steps. Attempts to direct electrons to one specific pathway over others have in general been failures and have highlighted the flexibility of metabolic fluxes in lower organisms. In most cases, only a small increase of products in the desired pathway is seen.

Based on preliminary data generated in their laboratory, the investigators proposed developing a system for studying the metabolic processes of phytosynthetic bacteria and “tunneling” the energized electrons from the photosystem directly into a redox-reactive site within the cell. If successful this would result in a photosynthetically-driven metabolism.

As proof of concept, the team will attempt to genetically modify photosynthetic microbes that have the ability to use CO_2 and N_2 from the atmosphere and produce hydrogen and oxygen using only solar energy. A major limitation to this approach is not the ability to tunnel the electrons, but rather the sensitivity of the enzyme that produces H_2, hydrogenase, to the oxygen produced during photosynthesis. Oxygen irreversibly inhibits hydrogenase activity at very low concentrations. To overcome the oxygen sensitivity of hydrogenase, the investigators have developed an *in vivo* selection scheme that will enable directed evolution of the hydrogenase gene. Current results show that hydrogenase mutants with increased oxygen tolerance can be obtained, thus validating the selection. Therefore an expanded effort in evolving oxygen tolerant hydrogenases will be pursued in the coming year and if successful will be an enormous advance in the field.

Coupling photosynthesis with hydrogen production will be an efficient means to provide a steady stream of energy in areas that are not easily accessible. Ultimately as development of this photosynthetic platform advances, it could be used to locally to efficiently synthesize a variety of useful, complex compounds.

D. Novel Thermostable, Highly-active Cellulases Using Structure-guided Recombination (SCHEMA)

Professor Francis Arnold, California Institute of Technology, ICB (UARC)

The goal of this project is to design and generate novel highly active, highly thermostable enzymes for incorporation into biofuel processes, to ultimately to allow fuels, such as JP-8, diesel and gasoline substitutes, to be produced from cellulosic biomass and wastes. Increasing the stability of such enzymes at higher temperatures, while retaining their catalytic activity for efficient biomass conversion, is a crucial step toward development of industrially relevant and affordable enzyme mixtures for biofuel production.

In previous Army-sponsored research, the Arnold group developed a novel set of computational tools to design synthetic cellulase enzymes (which break down cellulose into glucose) with high stability and activity, by recombining fragments of sequences from multiple parent genes isolated from fungi. One computational tool previously developed by the investigator is a computational algorithm called SCHEMA, which uses structural information to predict which fragments of related proteins can be swapped without disrupting the integrity of the three dimensional structure in different backgrounds. This algorithm has been shown to yield efficient, rapid results for predicting and creating novel cellulases, which are difficult to screen using high-throughput methods. Using SCHEMA, Professor Arnold has recombined fragments of highly active parent enzymes that are not necessarily thermostable, to create new sequences that fold into the same three-dimensional structure. This generates new enzymes that function at much higher temperatures, where cellulose accessibility and degradation are strongly enhanced.

Building upon this prior work, the investigators are now extending the model to predict and ultimately create novel highly active highly stable beta-glucosidase enzymes, to complement the improved cellulases produced to date. Beta-glucosidases are important because they reduce cellulase inhibition by cellobiose product and are needed for use in industrial cellulase mixtures. In addition to focusing on a new family of enzymes, the researchers are pursuing an innovative approach to recombine sequences from distantly related proteins (unlike the prior research focused on recombining sequences from closely related proteins) to increase the diversity of properties and functionality that can be achieved for the synthetic enzymes.

In the new approach, rather than being constrained to recombining amino acid sequences in a continuous fashion, the investigators are recombining sequence blocks that are non-continuous along the primary polypeptide chain and assemble in the three dimensional structure (see FIGURE 19). This opens up significant freedom in designing larger libraries of recombinant sequences with stability and functional diversity. Previous efforts in this project focused on recombinant libraries with continuous blocks because building a library with non-continuous blocks would have presented significant challenges in cloning DNA. However dramatic reductions in the cost of DNA synthesis will soon make individual synthesis cheaper than laborious and time-consuming DNA cloning of protein recombinant libraries.

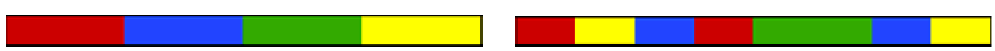


FIGURE 19

Example of protein sequence blocks for a 4-block library. The continuous blocks (left) and non-continuous blocks (right) are colored red, blue, green and yellow. In the continuous block case, each block is continuous along the polypeptide chain, while non-continuous blocks assemble in the 3D structure to form much stronger structural elements.

With these improved computational tools, it is anticipated that the group will build recombinant libraries of proteins from distantly related sequences. This will allow the investigators to choose from a greater number of potential parents, including those with interesting ranges of properties for recombination. This strategy also will increase the mutation level at a given level of protein disruption (see FIGURE 20) and will therefore enhance the potential for functional diversity. If successful it will be the first time that protein sequences from prokaryotic, eukaryotic and archaea domains have been recombined.

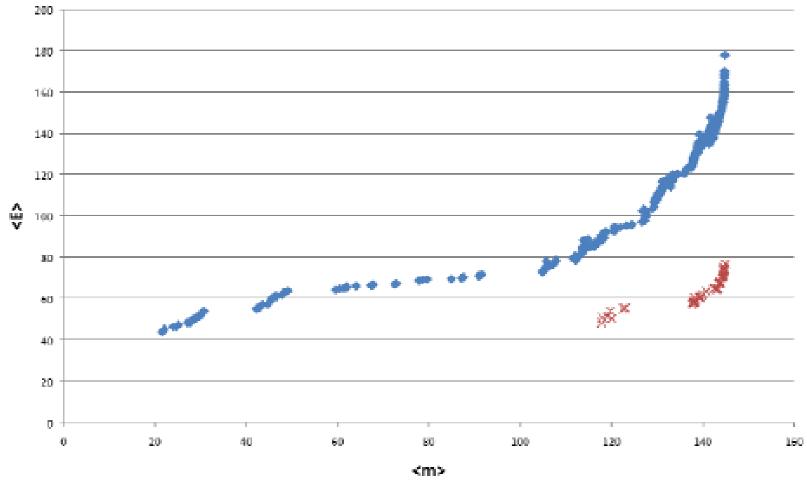


FIGURE 20

SCHEMA libraries from three parent GH1 beta-glucosidases. These libraries were designed with non-continuous blocks in red and continuous blocks in blue. For a given average number of mutations (x axis; <m>), the average SCHEMA disruption energy (y axis; <E>) of the non-continuous block libraries is substantially lower than the continuous block libraries.

Cellulases exhibiting high stabilities and high activities are needed for incorporation into a biofuel process, ultimately to allow fuels such as JP-8, diesel and gasoline substitutes to be produced from cellulosic biomass and wastes. This could ultimately reduce the supply train and associated costs for fuel delivery and will reduce reliance on foreign oil.

E. Investigating Cultural Consensus Theory Using Statistical Inference

Professor William Batchelder, University of California, Irvine

Culture is increasingly becoming an important concept in the conduct of Army operations. Although some may conceive of culture as monolithic or invariant, the extent to which cultural knowledge and beliefs can vary around a core set of shared understandings is important to consider. More importantly, the ability to measure culture and account for cultural variability is essential for understanding possible variations in human behavior.

This project is building the capacity for mathematically understanding culture at various levels of measurement (nominal, ordinal, and interval) that will enable more accurate models of culture that incorporate and better understand intracultural variation as well as comparisons across cultures. The researchers will meet this goal by employing an extension of an established formal model of culture from current limitations of multiple choice responses developed by the investigator to ordinal and interval level responses. The resulting tool will significantly advance our ability to mathematically model both intracultural and intercultural variation and their underlying causes (*e.g.*, religion, gender, the sexual division of labor).

F. Neurosensory Optimization of Information Transfer (NOIT)

Dr. Leonard Trejo, Pacific Development and Technology (PDT), LLC

The goal of this project is to develop a prototype system that filters a visual display to fit the unique capabilities of each cerebral hemisphere and dynamically compensate for changes in cognitive status, such as fatigue or cognitive overload. This development will build on recent advances by two ARO-supported teams. The UCLA team, led by Professor Zaidel, has developed new measures and models of lateralized attention networks, which allow a computer to match visual displays to processing resources in each hemisphere. The PDT team, led by Dr. Trejo, has developed robust algorithms for physiological estimation of cognitive status, which allow a computer to compensate for performance deficits arising from fatigue or overload by additional display filtering.

It is anticipated that the team will demonstrate a system that enhances and sustains human performance by continually filtering displays to match task demands and cognitive status. In addition it is expected that the

researchers will develop biofeedback methods that teach users self-control of hemispheric resources without the aid of external devices.

The ultimate application of this research is the development of portable, quick-setup hardware for EEG/EOG/EMG recording (refer to Section II-C.4 and F.1) for optimizing human cognitive processing. This system could ultimately include features for head-mounted eye-tracking, gaze-contingent, dual-camera monocular video system (for filtering different views of the task display to each hemifield), a PC-compatible interface, and custom software for dynamic allocation of hemifields and biofeedback training.

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CHAPTER 8: MATERIALS SCIENCE DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Materials Science Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize unprecedented materials properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army, with special emphasis on four Program Areas: Materials by Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. The objective of research supported by the Materials Science Division is to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. These research areas involve understanding fundamental processes and structures found in nature, as well as developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multicomponent systems such as composites, hierarchical materials and "smart materials" is of particular interest. Other important areas of interest include new approaches for materials processing, new composite formulations, and surface treatments that minimize environmental impacts, and novel composite concepts, including multifunctional and hierarchical materials. Finally, there is general interest by the Division in research programs to identify and fund basic research in the area of manufacturing science, which will address fundamental issues related to the reliability and cost (including environmental) associated with the production and long-term operation of Army systems.

2. Potential Applications. In addition to advancing and exploiting worldwide knowledge and understanding of new materials to achieve unprecedented properties, the research efforts managed by the Materials Science Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter and battlesystems. In the long term, the basic research discoveries made by ARO-supported materials research is expected to provide a broad base of disruptive and paradigm-shifting capabilities to address Army needs. Advanced materials will improve mobility, armaments, communications, personnel protection, and logistics support in the future. New materials will target previously identified Army needs for stronger, lightweight, durable, reliable, and less expensive materials and will provide the basis for future Army systems and devices. Breakthroughs will come as the fundamental understanding necessary to achieve multi-scale design of materials, control and engineering of defects, and integration of materials are developed.

3. Coordination with Other Divisions and Agencies. To realize the vision of the Materials Science Division and maximize transition and leverage of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, Reliance 21 Community of Interest for Materials and Processes), and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in pursuing other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

B. Program Areas

To meet the long-term program goals described in the previous section, the Materials Science Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Materials Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, and (iv) Synthesis and Processing of Materials. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Materials Design. The goal of the Materials Design Program Area is to enable the bottom-up design and fabrication of highly complex multifunctional materials with new and unprecedented properties (*e.g.*, negative index composites with optical cloaking properties or new classes of smart materials that can alter their behavior in response to environmental stimuli). In pursuit of this goal, this Program Area supports research that falls into three broad Thrusts: (i) Foundations for Future Directed Self-assembly of Materials, (ii) New Analytical Techniques for Characterizing Materials at the Nanoscale, and (iii) Understanding Complex Behavior that Emerges in Highly-coupled Systems (*i.e.*, studying frustration effects in magnetic systems, or better understanding field coupling effects in multiferroics). It is envisioned that the confluence of these Thrusts will culminate in the development of a new generation of engineered materials with new and unique capabilities. To realize this goal the program recognizes that the experimental program will require a strong complementary theoretical underpinning that addresses modeling of the relevant phenomenology, identification of robust pathways for directed self-assembly, and prediction/optimization of the final material properties.

Research supported under this Program Area is expected to provide materials that enable future disruptive capabilities and applications in communications, sensors, electronics, and logistics support. In addition, these efforts may enhance self assembly to affect property changes over time to introduce new properties, optimize performance, enhance reliability, and reduce cost and time to development.

2. Mechanical Behavior of Materials. This Program Area seeks to establish the fundamental relationships between the structure of materials and their mechanical properties as influenced by composition, processing, environment, and loading conditions. The program emphasizes research to develop innovative new materials with unprecedented mechanical and other complementary properties. Critical to these efforts is the need for new materials science theory that will enable robust predictive computational tools for the analysis and design of materials subjected to a wide range of specific loading conditions, particularly theory that departs from standard computer algorithms and is not dependent upon tremendous computational facilities. The primary research Thrusts of this Program Area are: (i) High Strain-rate Phenomena and (ii) Materials Enhancement Theory. The High Strain-rate Phenomena is focused on research to design new characterization methods and tools to elucidate the deformation behavior of materials exposed to high-strain rate and dynamic loading conditions, establish a detailed understanding of the physical mechanisms that govern this deformation, and realize novel mechanisms of energy absorption and dissipation. Materials Enhancement Theory focuses on developing a robust understanding of the interrelationships between materials processes and compositions and the range of properties that can be attained by them, particularly in terms of developing new materials theory capable of predicting such processing-property relationships and identifying novel mechanisms for enhancing specific toughness, engineering and synthesizing new materials containing unique and specifically designed chemical and biological functionalities and activities while maintaining, and preferably enhancing, requisite mechanical properties.

Research supported under this Program Area is anticipated to realize new materials that enable revolutionary capabilities in Soldier and systems protection, lightweight structural materials, predictive materials design theory, sensors, fuel cell membranes, and Soldier sustainment.

3. Physical Properties of Materials. This Program Area seeks to develop an understanding of the fundamental mechanisms responsible for the various physical properties (electronic, magnetic, optical, and thermal) of materials/composites through support of basic research that ultimately leads to development of future Army devices. General areas of research include modeling, innovative processing methods of materials with unprecedented physical properties, and novel characterization techniques for the determination of these physical properties. Three main Thrusts of this program are: (i) Defect Engineering of Advanced Materials, (ii) Materials for Thermal Management, and (iii) Novel 2D Free-standing Crystalline Materials. Defect Engineering of

Advanced Materials involves studies of semiconductors, ferroelectrics, superconductors, and others, and structures such as bulk materials, thin-films, and interfaces in advanced materials (*e.g.*, oxides, nitrides, carbon based materials). Materials for Thermal Management involves studies of novel thermal interface materials for thermal management of advanced electronics, carbon based materials, alloys, composites, as well as novel thermal property characterization methods. Novel 2D Free-standing Crystalline Materials includes fundamental research efforts with the goal of investigating the physical properties of novel free-standing crystalline 2D and composites of 2D/3D/1D materials (*e.g.*, oxides, nitrides), and characterizing unique properties/phenomenon in free-standing 2D crystalline materials.

These research Thrusts are expected to provide new materials that will address vital Army needs such as sensing, flexible displays, advanced electro-optical technologies, electronic materials/devices, advanced RF technologies, as well as power and energy (*e.g.*, micro, Soldier and portable power).

4. Synthesis and Processing of Materials. This Program Area focuses on the use of innovative approaches for processing high performance structural materials reliably and at lower costs. Emphasis is placed on the design and fabrication of new materials with specific microstructure, constitution, and properties. Research interests include experimental and theoretical modeling studies to understand the influence of fundamental parameters on phase formation, micro structural evolution, and the resulting properties, in order to predict and control materials structures at all scales ranging from atomic dimensions to macroscopic levels. The specific research Thrusts within this Program Area are: (i) Metastable Materials and Structures and (ii) Novel Processing Strategies. Metastable Materials and Structures focuses on (a) developing superior and affordable alloys, fibers, and composites with amorphous, ultra-fine grain, or otherwise highly controlled and meta-stable structures, (b) using *ab initio* theoretical approaches to design target electronic structures for functional moieties, and (c) synthesizing materials that exhibit these units to produce novel properties. Novel Processing Strategies supports research with the goals of (a) establishing and utilizing advanced and innovative processing approaches such as field enhanced processing, soft lithography, self-assembly, and bio-inspired and biomimetics, and (b) developing unique high strength alloys, metal matrix composites, and ceramic and polymeric composites, particularly those that offer enhanced repair or self-healing capabilities.

These research Thrusts are expected to provide new materials that will provide revolutionary solutions to the Army needs in the areas of: lightweight alloys and composites for vehicle structures, lightweight armaments, airframes, and bridging; advanced ceramics for improved armor; improved materials and processes for joining of components; high density metals for kinetic energy penetrators; fabrics and polymeric body armor; thermal and acoustical insulating foams; materials for gun tubes; and directed energy weapons.

C. Research Investment

The total funds managed by the ARO Materials Science Division for FY10 were $57.2 million. These funds were provided by multiple funding agencies and were applied to a variety of Program Areas, as described here. The FY10 ARO core (BH57) program funding allotment for this Division was $5 million. The Department of Defense Multi-disciplinary University Research Initiative (MURI), Defense University Research Instrumentation Program (DURIP) provided $11.1 million to programs managed by the Materials Science Division. The Division also managed $38.9 million from the Defense Advanced Research Projects Agency (DARPA). The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.38 million in FY10. In addition, congressional earmarks provided $1.2 million. Finally, $0.67 million was provided in FY10 for use by the Presidential Early Career Award for Scientists and Engineers (PECASE) and the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) programs.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Armor Ceramic Symposium (Daytona Beach, FL; 24-29 January 2010). The goal of this symposium was to discuss new ideas and needs pertaining to the development and incorporation of ceramic materials for armor applications. Specific topics covered at the symposium included: transparent materials (*e.g.*, transparent armor systems, missile windows and radar dome (radome) applications, and impact resistant glass systems, cost effective surface treatments, and adhesives), dynamic behavior (*e.g.*, damage characterization, inelasticity and failure mechanisms, static and dynamic property testing, shock wave/blast effects, and surface effects), boron carbide (*e.g.*, concepts, processes, and characterization), as well as impact, penetration, and material modeling (*e.g.*, particle mechanics, multi-scale, micro- and meso-structural, and incorporation of flaws and inelasticity mechanisms).

2. Biological Materials Science Symposium (Seattle, WA; 14-18 February 2010). The goal of this symposium was to provide a unique venue for research discussions and explorations at the intersection of materials science and biology. The symposium specifically focused on: bio-inspired materials design and processing, mechanical behavior of biological materials, surface engineering, and computational materials science. The meeting provided extremely high value to the participants, their organizations, and the national technical community by bringing together individuals from academia, government, and industry.

3. 6th International Symposium on Ultrafine Grained Materials (Seattle, WA; 14-18 February 2010). The goal of this symposium was to provide a venue for new research discussions and explorations in the area of ultrafine-grained materials. The symposium brought increased attention to ultrafine-grained (UFG) materials with grain sizes in the range from 10 to 1000 nm. In particular, the relatively high strengths of bulk UFG materials (*i.e.*, typically 5-10 times that of conventional materials of similar composition), and the ability to produce bulk UFG materials free of porosity and of dimensions suitable for structural applications, have provided significant motivation for exploration of these novel materials.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant

portion of the basic research programs managed by the Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. Single Nuclear Spin Detection. This MURI began in FY05 and was granted to a team led by Professor John Sidles at the University of Washington. The objective of this MURI is to provide a proof-of-concept demonstration that continued development of magnetic resonance force microscopy (MRFM) can lead to *in situ* detection of individual nuclear magnetic moments and three-dimensional mapping of their positions with atomic resolution.

Fundamental scientific and engineering studies involving multiple disciplines are being conducted in an effort to design and construct a system capable of detecting single nuclear spins. The specific goals of this project are to pursue studies in (i) fundamental spin physics and noise mechanisms to identify a valid design path and the operative quantum design rules, (ii) system engineering, to include design and fabrication of acoustic and MHz Larmor cantilevers with high field-gradient magnetic tips and high resolution position monitoring, (iii) the development of optimal system control and noise minimization procedures, (iv) the establishment of data collection protocols and image reconstruction procedures for efficient signal processing, and (v) 3D imaging trials to validate performance metrics and demonstrate integrated system capabilities. This research has the potential to revolutionize the fields of nanotechnology and biotechnology by providing unsurpassed capability to map both the chemistry and local structure of molecular assemblies with atomic resolution.

2. Studying Underlying Principles of Large Lattice Mismatched Materials. This MURI began in FY05 and was granted to a team led by Professor Thomas Kuech at the University of Wisconsin. The objective of this research is to develop the science base and infrastructure needed to engineer new device structures based on the heteroepitaxial growth and layer transfer of lattice mismatched semiconductor films.

More specifically, the goals of this research are to (i) conduct heteroepitaxial growth studies complemented with theoretical modeling to identify approaches for controlling defect nucleation, motion and reduction in lattice mismatched systems, (ii) develop techniques for the liftoff, transfer and bonding of semiconductor layers as an alternative approach to materials integration, (iii) engineer the strain state of the film to expand miscibility limits or enhance electrical performance, and (iv) demonstrate novel device structures and prototype devices that build on the new breakthroughs in materials integration.

3. Investigating Superatoms as Building Block of New Materials. This MURI began in FY06 and was granted to a team led by Professor A. Welford Castleman at the Pennsylvania State University. The objectives of this research are to (i) synthesize atomic clusters of tailored composition, structure, and size, and (ii) self-assemble these clusters into condensed films and solids at the micrometer length scale that retain the distinct properties of the clusters.

The electronic structure of small clusters of free-electron metallic and metalloid atoms is fundamentally different from the bulk. This gives unique "superatom" bonding properties to these clusters that resemble atomic bonding, but are distinctly different in character from any of the elements, which could result in novel properties for assembled solids formed of these clusters. Once assembled into solids, the objective is to characterize the mechanical and electro-optical properties of the films and solids and compare them to the current theoretical understanding of these systems. This should validate the current theoretical understanding and lead to sufficient model fidelity to begin activities on the exploration of devices based on cluster materials. Exploration of these materials is only just beginning and, aside from the C_{60}-based materials, assembled cluster solids at this scale are unknown. A number of significant contributions could be achieved if the research team is successful in developing synthesis routes for different classes of clusters into macroscopic specimens, analogous to fullerenes, as proposed. Since the available variables are greatly extended by exploration of the periodic table beyond carbon, the properties of the clusters could be tailored for device requirements with electronic and optical devices expected to be the first applications of the science to technology.

4. Characterizing Ionic Liquids in Electro-active Devices (ILED). This MURI began in FY07 and was granted to a team led by Professor Timothy Long at the Virginia Polytechnic Institute and State University (Virginia Tech). The goal of this MURI is to use ionic liquids both as a reaction medium for synthesizing polymers, as an active component incorporated into the final polymer structure, and to fabricate and characterize new actuator devices with dramatically improved performance. This program is co-managed with the ARO Chemical Sciences Division.

Electroactive materials are materials that exhibit a physical response, usually a change in shape, under activation by an electrical potential. These materials are useful in a number of applications including MEMS, stimuli-responsive structures, energy harvesting, micro-sensors, chem-bio protection, and portable power. The main technological limitations of these materials, which limit their usefulness, are their relatively slow response time and low actuation authority (the maximum force they can apply). The focus of the research is on molecular design, synthetic methodology, nanoscale morphological control, property measurements, modeling, and characterization of device performance. The specific research areas of this project include the study of (i) free radical, step growth, and condensation, (ii) polymer structure characterization using atomic force microscopy (AFM), scanning transmission electron microscopy (STEM), small angle X-ray scattering (SAXS), dynamic mechanical analysis (DMA), transmission electron microscopy (TEM), and standard polymer characterization techniques, such as nuclear magnetic resonance (NMR) and gel permeation chromatography (GPC), (iii) the synthesis of zwitterionic monomers using step- and chain-growth polymerizations to form membranes and crosslinked networks, and (iv) the synthesis and characterization of liquid crystalline monomers containing imidazolium sites.

5. Materials on the Brink: Unprecedented Transforming Materials. This MURI began in FY07 and was granted to a team led by Professor Kaushik Bhattacharya at the California Institute of Technology. The objective of this research is to develop a fundamental understanding and establish the engineering expertise needed to tailor the electrical, optical, or magnetic (EMO) properties of phase transforming materials through the design and implementation of highly reversible, phase-transformations.

This research is investigating different approaches to achieving highly reversible phase transformations, including such effects as engineered phase compatibility and frustration. The broad selection of material systems (perovskites and multi-ferroics, Heusler alloys, SMA, and oxy-acid proton conductors), and the design of the studies, will develop a fundamental understanding of the underlying physics that developers need to predict the occurrence of states and the range of behaviors that can be realized within engineered phase transforming materials. The specific goals of this project are to develop and characterize (i) perovskites for electrically tunable photonics and RF-to-optical converters, (ii) metal-ferroelectric multilayers for negative refractive index material applications (a negative surface-plasmon polariton was shown to provide NIM behavior in the visible part of the spectrum), light modulators, thermo-magnetic cooling, spintronics and magnetic field sensing, (iii) shape-memory alloys for large-strain actuators, and (iv) proton-conducting electrolytes for fuel cells. New strategies based on phase engineering of materials have been successfully realized in actuation systems (*e.g.*, in shape memory alloys and relaxor ferroelectrics). These same underlying principles may ultimately be transferable to the development of EM sensors, tunable phase shifters, adaptive optics, optical limiting and energy harvesting devices for use by the Army.

6. Spin-Mediated Coupling in Hybrid Magnetic, Organic, and Oxide Structures and Devices. This MURI began in FY08 and was granted to a team led by Professor Michael Flatte at the University of Iowa. The objectives of this research are to (i) improve the field's understanding of spin behavior in hybrid systems where magnetic semiconductors and/or organics are integrated with ferromagnetic metals and multiferroic oxides, and (ii) develop the engineering expertise needed to exploit spin -mediated processes to establish nanoscale control over the spin transport, local magnetic order, and electrical/optical/magnetic properties of hybrid magnetic systems.

More specifically, the goals of this project are to (i) investigate, both experimentally and theoretically, spin behavior and magnetic field manipulation in hybrid magnetic systems, (ii) develop a fundamental understanding of the physics involved in spin current generation and control, spin momentum transfer, and magnetic field manipulation, (iii) establish techniques for controlling dynamic spin phenomena in nanoscale systems, including both isolated nanomagnets and nanomagnetic arrays, and (iv) design and fabricate device structures that utilize spin polarization currents and momentum transfer as a means of attaining new functionality and capabilities. The research may lead to novel electronic devices that include: circularly polarized light emitting diodes, lasers and detectors, nanoscale microwave and millimeter wave oscillators for signal processing and chip-to-chip communications, reconfigurable circuitry, smart sensors for IED detection, and spin-based logic processing (including quantum computing) for data manipulation and computing.

7. Design of Adaptive Load Mitigating Materials Using Nonlinear Stress Wave Tailoring. This MURI began in FY09 and was granted to a team led by Professor John Lambros at the University of Illinois, Urbana.

This research is focused on understanding and exploiting wave tailoring phenomena in highly nonlinear inhomogeneous granular media.

The effort builds on recent results demonstrating remarkable dynamic properties in such media, including tunability, energy trapping and wave redirection, primarily because of the highly nonlinear forces that are generated during contact of the granular crystals. Specific granular microstructures will be designed to fully exploit the nonlinear contact effect. Additionally, novel phase transforming ceramics will be fabricated that enhance the granular materials properties by, for example, preferentially strengthening or weakening the material to control local energy dissipation. More specifically, the goals of this research effort are to (i) incorporate a granular medium in the material system in order to introduce nonlinearity in the material microstructure through local contact between material “elements”, thereby furnishing an adaptive and nonlinear targeted energy transfer (TET) capability, (ii) provide additional adaptively coupled with enhanced energy absorption by developing new phase transforming ceramics, (iii) arrange these and other elements in a material system that is either layered (2D), or integrated with a 3D microstructural architecture, and (iv) utilize geopolymers (polymer-like ceramics) to create interfaces that join constituents and also act as “traditional” wave arrestors or reflectors. The comprehensive understanding of propagation and mitigation of high-pressure stress-waves in complex media will guide the future design and demonstration of new materials optimized for high-strain-rate ballistic performance, particularly armor materials. The research is expected to enable lightweight military hardware with dramatically enhanced survivability to serve the Soldier in the battlespace of the future, in addition to new paradigms for insensitive munitions.

8. Innovative Design and Processing of Multi-functional Adaptive Structural Materials. This MURI began in FY09 and was granted to a team led by Professor Ilhan Aksay at Princeton University. The objective of this research is to develop innovative processing techniques for the design and modeling of hierarchically porous adaptive structures that are optimized for strength and transport and that support multiple functions ranging from biosensing and catalysis to self healing.

The effort focuses on sensing stress variations on the struts of cellular or porous structures and responding with mass deposition at those sites to negate the weakening effect of the increased stress. More specifically, the goals of this research effort are to (i) understand the dispersion and percolation characteristics of FGS in the solutions, (ii) understand the mechanisms of conduction with FGS-filled coatings, (iii) optimize the multifunctionality of the composites with respect to mechanical properties (*e.g.*, stiffness, strength, thermal stability, radiation resistance, and dimensional stability with water and solvents), (iv) maximize the conductivity of individual FGS by regulating its C/O ration through heat treatment, and (v) understand and minimize the effects of contact resistance between the sheets. This research effort may lead to significant innovations in the design and integration of adaptive materials, which would lead to substantial contributions to DoD missions. Specifically, the research is expected to produce novel systems with multiple functions that include catalysis, self-healing, heat transport, and energy production.

9. Reconfigurable Matter from Programmable Colloids. This MURI began in FY10 and was granted to a team led by Professor Sharon Glotzer at the University of Michigan. The goal of this MURI is to enable the design and synthesis of an entirely new class of self-assembled, reconfigurable colloidal material capable of producing materials with radically increased complexity and functionality.

Opportunities for manipulating the assembly process include the utilization of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site specific binding groups, molecule-to-substrate interactions, and external fields. Pathways including both sequential assembly and selective disassembly processes are to be investigated. One goal of this research effort is to establish an ability to selectively disassemble and reconfigure these pathways through judicious exposure to heat, pH or light. The research also includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research approaches include the sequential staged self-assembly of nano-particles into complex and hierarchical architectures, the development of theoretical tools and computational algorithms to model the self-assembly process, identification of stable self assembly pathways that lead to the targeted hierarchical structures, and finally prediction of the final properties of the assembled material. Ultimately the research will focus on the derivation of tailored properties and functions within highly complex or hierarchical materials. This research effort may ultimately revolutionize the materials capabilities for building increasingly complex, functional materials of the future.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY10.

E. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY10.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Advanced Cut Studies and Fracture Toughness of Single Fibers. This TCU project is led by Professor Shaik Jeelani at the Tuskegee University of Puerto Rico to explore and establish the fundamentals of fiber mechanics in structural fibers during cutting.

The research focuses on three specific objectives. First, the researchers are seeking to obtain fracture toughness data for single fiber samples. Sample materials will include Kevlar, Twaron, Dyneema, Zylon, Vectran, Technora, S2-glass and carbon fiber, and will address both single and mixed modes of failure. Computational models that incorporate these effects will also be explored and compared to experimental work. Fracture toughness of anisotropic materials will be investigated (*i.e.*, fibers with a morphology that varies from center to surface). Single-fiber testing will be conducted with use of a specially designed test stage that enables in-situ experiments and observations of tensile and fracture toughness testing. Second, the effort will seek to determine the relationship between single fiber fracture toughness and yarn mechanical properties governing complex deformation and failure resistance (*i.e.*, cut/puncture, high-rate deformation). The physical mechanisms of cut failure will be examined through an array of characterization and imaging tools, and the effect of filament coatings will be investigated. Third, the proposed research will seek to relate single fiber fracture toughness to yarn strength. The tensile mechanics of single fibers will be thoroughly analyzed and characterized and a statistical analysis will be conducted to identify differences between single fiber and yarn mechanics. Experimental testing and microscopy will also be incorporated in order to elucidate the mechanisms and phenomena governing deviations between single fiber and yarn strengths of Kevlar fiber.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Materials Science Division managed six new DURIP projects, totaling $0.97 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies to provide new capabilities for materials characterization and stress wave mitigation, to develop robust property maps for a broad range of synthetic and biological materials, and to optimize the design of novel multiferroic materials.

I. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in

the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

J. DARPA Bioinspired Photonics (BIP) Program

The goal of the DARPA BIP program is to harness innovative bioinspired synthetic organic and inorganic approaches to drive improved photonic material capabilities. Nature's hierarchical structures, scaling from micron to nanometer level, achieve remarkable optical functionality through complex scattering, reflection and absorption phenomena. The Bioinspired Photonics program draws inspiration from the best of nature's photonic structures to demonstrate tunable reflectors and volatile organic vapor sensors capable of operating in the visible and near infrared. The Materials Science Division currently co-manages projects within this program with the goal of identifying new approaches to the design and fabrication of future high performance photonic systems.

K. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

L. DARPA Advanced Structural Fiber (ASF) Program

The goal of the ASF program is to develop and produce a fiber that offers at least a 50-percent increase in strength and stiffness. The ASF program is focused on exploiting recent breakthroughs in the understanding of materials synthesis at the atomic level, new materials characterization techniques, and advanced fiber manufacturing processes to scale up production fiber technologies that have already shown revolutionary lab-scale results. The Materials Science Division currently co-manages projects within this program seeking to explore and optimize the most promising fiber compositions and processing strategies and to establish new paradigms for revolutionary fiber precursors.

M. DARPA Chemical Communications Program

The Chemical Communications program is exploring innovative methods to develop self-powered chemical systems that can encode an input string of alphanumeric characters (*i.e.*, a message), convert the message to a modulated optical signal, and transmit it repetitively to a receiver. The ultimate goal of this program is to develop a small replicator device, with the form factor of a personal digital assistant or cell phone that will enable warfighters to generate disposable optical transmitters in real time, each with a user-specified message. The Materials Science Division currently co-manages projects within this program exploring various chemical phenomena capable of generating unique approaches to optical transmissions and communications.

N. DARPA Chemical Robots (ChemBots) Program

The goal of the ChemBots program is to create a new class of soft, flexible, mesoscale mobile objects that can identify and maneuver through openings smaller than their dimensions and perform various tasks. The program seeks to create a convergence between materials chemistry and robotics through the application of any one of a number of approaches, including gel-solid phase transitions, electro- and magneto-rheological materials, geometric transitions, and reversible chemical and/or particle association and dissociation. The Materials Science Division currently co-manages projects within this program seeking to demonstrate a new functional form of matter to enable an entirely new approach to robotic sensing and data collection.

O. DARPA Feedback Regulated Automatic Molecular Release Program

The goal of the DAPRA Feedback Regulated Automatic Molecular Release program is to develop biodegradable self-regulating drug delivery systems that enable feedback-regulated release in response to a biomarker(s) correlated with drug efficacy and/or toxicity. These systems will enable Soldier self-care through the development of drug delivery methods that assure, in the combat environment, the delivery of a therapeutic dose while eliminating the possibility of drug overdose. Delivery systems for one or more of the therapeutics classes that are currently used in tactical field care or battlefield medicine are of particular interest. The early objectives of this project are to demonstrate that the release rate of the drug from the new system is sufficient to achieve therapeutic levels, but can be reduced by an amount sufficient to avoid toxicity (*e.g.*, >10:1) in the presence of a biomarker correlated to a toxic effect. The Materials Science Division currently co-manages projects within this program seeking to realize novel approaches to battlefield drug delivery systems based upon novel molecular structures and materials architectures.

P. DARPA Fracture Putty Program

The DARPA Fracture Putty program seeks to create a dynamic putty-like material which, when packed in/around a compound bone fracture, provides full load-bearing capabilities within days, creates an osteoconductive bone-like internal structure, and degrades over time to harmless resorbable by-products as normal bone regenerates. This new material could rapidly restore a patient to ambulatory function while normal healing ensues, with dramatically reduced rehabilitation time and the elimination of infection and secondary fractures. The Materials Science Division currently co-manages projects within this program attempting to achieve a convergence of materials science, mechanics, and orthopedics to enable new paradigms in bone stabilization, growth, and regeneration.

Q. DARPA Instant Fire Suppression (IFS) Program

The DARPA IFS program seeks to establish the feasibility of a novel flame-suppression system based on destabilization of flame plasma with electromagnetic fields, acoustics, ion injection or other novel approaches. The key to transformative firefighting approaches may lie in the fundamental understanding of fire itself. Fire suppression technologies have largely focused on disrupting the chemical reactions involved in combustion. Yet from a physics point of view, flames are cold plasmas consisting of mobile electrons and slower positive ions, and by using physics techniques rather than combustion chemistry, it may be possible to extinguish and/or manipulate flames. To achieve this goal, key scientific breakthroughs are needed to understand and quantify the interaction of electromagnetic and acoustic waves with the plasma in a flame. IFS research results will be used to determine the scalability of potential techniques, and if scaling is achievable, the program will design and construct a prototype fire suppression system for Class A and B fires inside of a ship or HUMVEE-sized compartment. The Materials Science Division currently co-manages a project within this program seeking to understand and demonstrate new paradigms for flame suppression and control.

R. DARPA Plasma Sterilization of Wounds and Medical Devices Program

The DARPA Plasma Sterilization program is investigating the ability of a plasma, or partially ionized gas, to kill pathogenic bacteria on the surface of the skin, thereby leading to improved wound healing outcomes and reduction of secondary infections. Preliminary research has indicated that a non-thermal, atmospheric pressure plasma can drastically reduce the population of a wide range of pathogenic bacteria placed on skin surrogates in controlled experiments. By investigating how these results translate to living skin, the program will build the foundation for a novel medical technology. The Materials Science Division currently co-manages a project within this program seeking to assess and enhance the mitigating effects of plasma on bacterial infections.

S. DARPA PowerSwim Program

The DARPA PowerSwim program is developing highly efficient, human-powered swimming devices for use by combat and reconnaissance swimmers. This program explores a new concept in swimming propulsion that uses

the same oscillating foil approach to swimming that is exhibited by many fish and aquatic birds. This propulsion approach is more than 80-percent efficient in conversion of human motion to forward propulsion. Typical recreational swim fins are no more than 15-percent efficient in their conversion of human exertion to propulsive power. This dramatic improvement in swimming efficiency will enable subsurface swimmers to move up to two times faster than is currently possible, thus improving swimmer performance, safety, and range. The Materials Science Division currently co-manages a project within this program exploring novel materials and designs to provide revolutionary enhancements to the swimming propulsive efficiency of combat swimmers.

T. DARPA Programmable Matter Program

The goal of the DARPA Programmable Matter program is to demonstrate a new functional form of matter, based on mesoscale particles, which can reversibly assemble into complex 3D objects upon external command. These 3D objects will exhibit all the functionality of their conventional counterparts. Programmable Matter represents the convergence of chemistry, information theory, and control into a new materials design paradigm referred to as "InfoChemistry" - building information directly into materials. Of critical importance are radical new material architectures that maximize the efficiency of information processing/transfer, and design rules for the optimal number, size, and shape of particles required to create objects of a specific size and spatial feature resolution. The Materials Science Division currently co-manages projects within this program exploring a wide range of materials systems, compositions, and structures to provide reversible assembly and robust control.

U. DARPA Revolutionizing Prosthetics Program

The DARPA Revolutionizing Prosthetics program will create, within this decade, a fully functional (motor and sensory) upper limb that responds to direct neural control. This revolution will occur by capitalizing on previous DARPA investments in neuroscience, robotics, sensors, power systems, and actuation. DARPA has delivered a prosthetic for pre-clinical trials that is far more advanced than any device currently available. This prosthetic enables many degrees of freedom for grasping and other hand functions, and will be rugged and resilient to environmental factors. The program now seeks to deliver a prosthetic for clinical trials that has function almost identical to a natural limb in terms of motor control and dexterity, sensory feedback (including proprioception), weight, and environmental resilience. The results of this program will allow upper limb amputees to have as normal a life as possible despite their severe injuries. The ARO Materials Science and Life Sciences Divisions currently co-manage a project within this program with the goal of optimizing materials and controling architectures to realize maximum capabilities in upper-arm prostheses.

V. DARPA Structural Logic Program

The DARPA Structural Logic program seeks to enable structural systems that make up the basis for modern military platforms and buildings to adapt to varying loads and simultaneously exhibit both high stiffness and high damping. By demonstrating the ability to combine stiffness, damping, and adaptive dynamic range in a single structure, the Structural Logic program will enable the design of military platforms with the ability to continually change their properties to match the demands of a broad range of dynamic environments. The Materials Science Division currently co-manages projects within this program seeking to realize novel design paradigms for passively adaptive structural systems that combine high stiffness, damping, and unprecedented adaptability.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Materials Science Division.

A. Laser Integration into Si Integrated Circuits

Professor Luke Mawst, University of Wisconsin, and Professor Nan Jokerst, Duke University, MURI Award

The objective of this effort is to provide a comprehensive understanding of growth, integration and fabrication related to large lattice mismatched material systems. The research seeks identify growth and integration techniques that yield low defect densities in large lattice-mismatched epitaxial systems, and includes a variety of approaches for controlling the nucleation and enhancing the mobility of dislocations in epitaxially grown layers.

This team of researchers recently demonstrated a device lift-off and integration technology, which is appropriate for inserting III-V laser structures into an Si integrated circuit (IC), that roughly doubles the power efficiency and data transmission compared to alternative heteroepitaxial growth approaches. This research revealed that incorporating strain compensating strategies during the growth of the edge emitting laser structures the devices could be detached from their native substrates and transferred onto Si platforms. This property avoids the problem of material performance degradation that is experienced when various material overlayers are grown on substrates that have even small lattice misfits. Superior device performance is possible since both the top and bottom surfaces of the device are made accessible during various stages of processing. This access permits design changes that enhance optical and current confinement, and provide improved thermal management solutions. These improved designs led to record low threshold currents (260 A/cm^2) in devices that were heat sunk to broad metal pads for heat dissipation. Finally, an overlapping waveguide design was developed to integrate the laser into the Si IC (see FIGURE 1). This approach resulted in excellent waveguide coupling efficiencies and misalignment tolerance. The waveguide integration resulted in a moderate degradation in laser gain due to reduced facet reflection; however, the final assembly displayed very low threshold currents in the range of 320 A/cm^2.

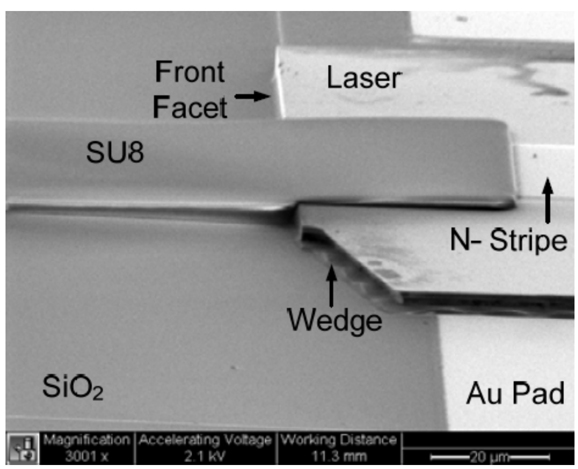

FIGURE 1

Laser-integrated Si IC. This scanning electron microscope (SEM) image shows an InGaAs/GaAs edge emitting laser integrated with a polymer waveguide on a Si substrate.

B. Shaping Nanocrystals with Biomolecular Specificity

Professor Yu Huang, University of California, Los Angeles (UCLA), PECASE Award

The objective of this project is to demonstrate a rational approach to the synthesis of nanocrystals with predictably controlled surfaces and morphologies using biologically evolved peptides as a molecular regulating agent. The project utilizes biomolecular specificity to synthesize highly active and selective inorganic

nanocatalysts, and to integrate them with semiconductors. Once optimized, peptide sequences will be used as modulating agents to regulate the synthesis of Pt nanocatalysts with selectively exposed catalytic surfaces.

Researchers at UCLA have found that biomolecules possess exquisite specific molecular recognition properties that can be used for the precision engineering of nanostructured materials in aqueous solutions. More specifically, the investigators have recently demonstrated that facet-specific peptide sequences can be utilized as a regulating agent for the room temperature synthesis of platinum nanocrystals with predictable exposed crystal surfaces and shapes. The team was able to identify appropriate Pt-{100} and Pt-{111} binding peptide sequences by adopting a biomimetic evolution process. The research then demonstrated that these facet-specific peptides could be used to direct the growth of Pt nanocrystals in a highly predictable manner. For example, the presence of Pt-{100} binding peptides produced cubes enclosed by six {100} facets and the presence of Pt-{111} binding peptides produced tetrahedrons enclosed by four {111} facets. Furthermore, the researchers were able to drive a shape transformation from cube to tetrahedron by replacing the {100} binding peptide with a {111} binding peptide in the solution. According to the lattice spacing measurement, the spacing distance of 2.26 Å is corresponding to the {111} lattice spacing, which means that the pods are growing along {111} direction with the presence of peptide in solution. With increasing peptide concentration, nanocrystals show shorter lengths along the{111} direction and more nanocrystals emerge as bipods (see FIGURE 2). These studies demonstrate unambiguously the abilities of the facet-selective binding peptides to control the nanocrystal shapes, presenting a critical step forward in exploiting biomolecules for programmable synthesis of nanostructures.

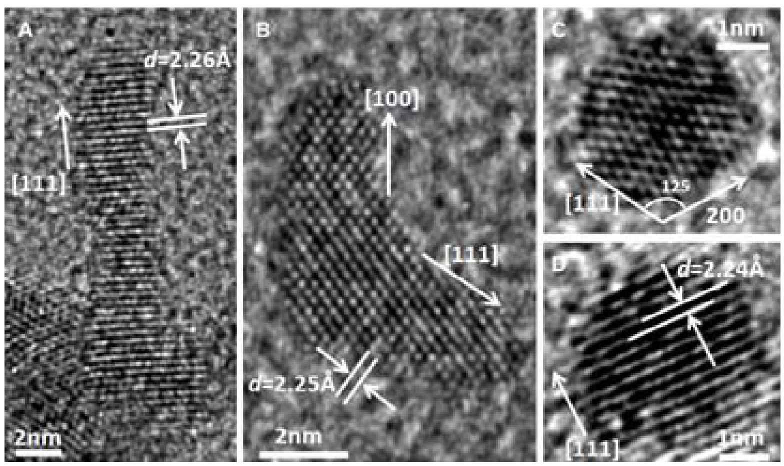

FIGURE 2

Increasing peptide concentration changes lattice spacing. Facet-specific peptides were used to direct the growth of Pt nanocrystals in a highly predictable manner. HRTEM images of crystals synthesized from reactions with peptide concentrations of (**A**) 20, (**B**) 25, and (**C-D**) 250 μg/mL.

C. Corrosion Resistant High-Conductivity Alloys

Professor Pamir Alpay, University of Connecticut, Single Investigator Award

High contact resistance is a common cause of device/system failure in aggressive environments, as 43% of all electrical failures are due to contacts. Novel contact materials are needed to improve device reliability and reduce asset loss due to electrical failure in various Army applications. The objective of this project is to develop novel electrical contact materials through studies of alloy design. Several mechanisms were investigated to improve the base metal performance (*i.e.*, to reduce the contact resistance), including (i) doping, (ii) developing a conductive vein structure, (iii) polaron hopping, and (iv) two-phase conductive metal-oxide mixtures.

New alloy designs were found to form corrosion resistant, self-healing and inherently conductive oxide scales when exposed to aggressive environments (such as desert battlefields) and thereby maintain low contact resistance. In addition to potential uses in electrical circuitry, the alloys could be used in the development of interconnects, sensors, and non-noble-metal catalysts.

This research recently led to significant breakthroughs, including the development of two systems: a Fe-V system with four orders of magnitude improvement over pure Cu and approximately two orders of magnitude

improvement over Fe, and a Ni-Ru system with seven orders of magnitude improvement over pure Cu and three orders of magnitude improvement over pure Ni (see FIGURE 3). Efforts are underway to commercialize and further improve these materials in collaboration with United Technologies Research Center (UTRC).

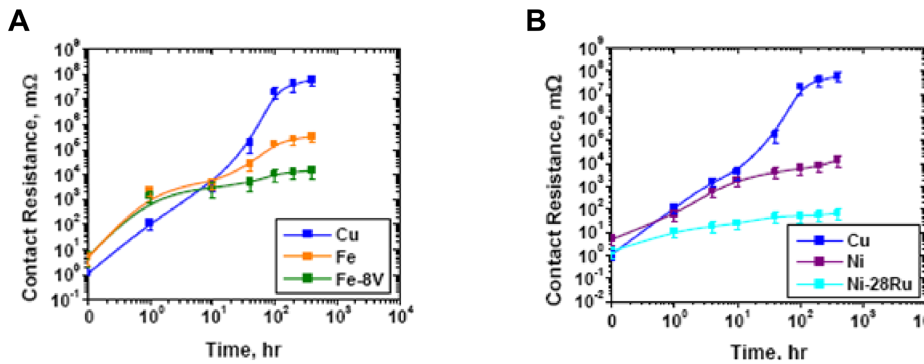

FIGURE 3

Contact resistance of new alloys as a function of oxidation time. This research effort resulted in the development of (A) a Fe-V system with four orders of magnitude improvement over pure Cu and approximately two orders of magnitude improvement over Fe, and (B) a Ni-Ru system with seven orders of magnitude improvement over pure Cu and three orders of magnitude improvement over pure Ni.

D. Thermo-magnetic Thermoelectric Materials

Professors Hariharan Srikanth and George Nolas, University of South Florida, Single Investigator Award

The objective of this project is to investigate the mechanisms to develop a dual-mode thermo-magnetic and thermoelectric material system that can be used for low temperature cooling. $Eu_8Ga_{16}Ge_{30}$ clathrates were investigated as the host matrix materials as they serve as excellent thermoelectric refrigerant systems at high temperature (T > 200 K). Systematic chemical substitutions of rare-earth dopants and second phase additions were employed to stabilize and tune the magneto-caloric effect in the low to intermediate temperature range of 20-100 K (see FIGURE 4).

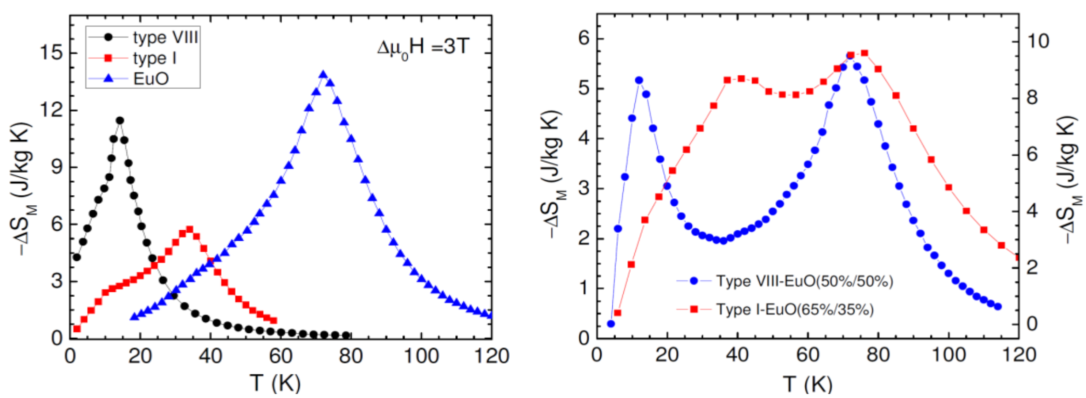

FIGURE 4

Representative plots of magnetic entropy changes ($-\Delta S_M$) of various materials.

This research revealed that $Eu_8Ga_{16}Ge_{30}$ type-VIII clathrates ($-\Delta S_M$ = 11.4 J/kg K at 3T) show reversible giant magnetocaloric effect. It was also found that by doping with non-magnetic elements like Sr, magnetic ordering, the magnetocaloric effect and refrigeration capacity in $Eu_8Ga_{16}Ge_{30}$ type-I clathrates can be tuned. A very large refrigeration capacity of 760 J/kg at 6T over a 80 K interval in Type I clathrate-EuO composites (65%/35%) was observed. In addition, a potential of using composite materials to produce refrigeration in two different temperature ranges was demonstrated as well. For example, Type VIII clathrate-EuO composites (50%/50%) show two distinct magnetocaloric effect peaks at 15 K and 77 K. The long-term Army-relevant applications of this work are efficient cooling technologies for IR night vision equipment as well temperature stabilization of advanced electronics and lasers.

E. Enhanced Microstructural Stability and Deformation Behavior in Tantalum Carbides

Professor Gregory Thompson, University of Alabama, Single Investigator Award

One of the significant challenges of utilizing tantalum carbides (Ta_xC_{1-x}) and other similar refractory compounds is their high melting points. Though advantageous for ultrahigh temperature applications, the difficulty in production of fully dense, near net shape structures limits the ability for easy manufacturing. This project investigates the γ-TaC phase, which has a melting temperature near 4,000 ^oC. The precipitation of substoichiometric Ta-rich phases, such as α/β-Ta_2C and ξ-Ta_4C_3, with similar high melting points, provides ample opportunities to tailor the microstructure for improved thermomechanical behavior.

The researchers investigated a series of $Ta_{53}C_{47}$, $Ta_{55}C_{45}$, and $Ta_{63}C_{37}$ specimens. In the $Ta_{53}C_{47}$ VPS as-sprayed condition, a distribution of grain sizes and phases existed. Upon the subsequent sintering, the grain size became uniform and equiaxed. The post-VPS processing also homogenized the phase content to be single phase TaC. Upon fabricating specimens with less carbon content, the precipitation and stabilization of Ta_4C_3 and Ta_2C was secured. For the $Ta_{55}C_{45}$ specimen, an equiaxed grain structure with secondary phases of Ta_4C_3 precipitated on multiple variants of {111} (see Figure 5a). The $Ta_{63}C_{37}$ specimen exhibited an acicular grain morphology (see Figure 5b). The precipitation of Ta_4C_3 and Ta_2C was found to be parallel to the major-axis of the acicular grain with each grain consisting of multiple stacking of these secondary phases. These phases also spanned the entire length of the major axis direction of the acicular grain. Based upon the low lattice misfit for the orientation relationship between these phases and TaC, these low interfacial energy planes dominate which consequently yield an anisotropic growth direction that changes the grain morphology from equiaxed to acicular with increasing volume fraction of the secondary phase content within TaC.

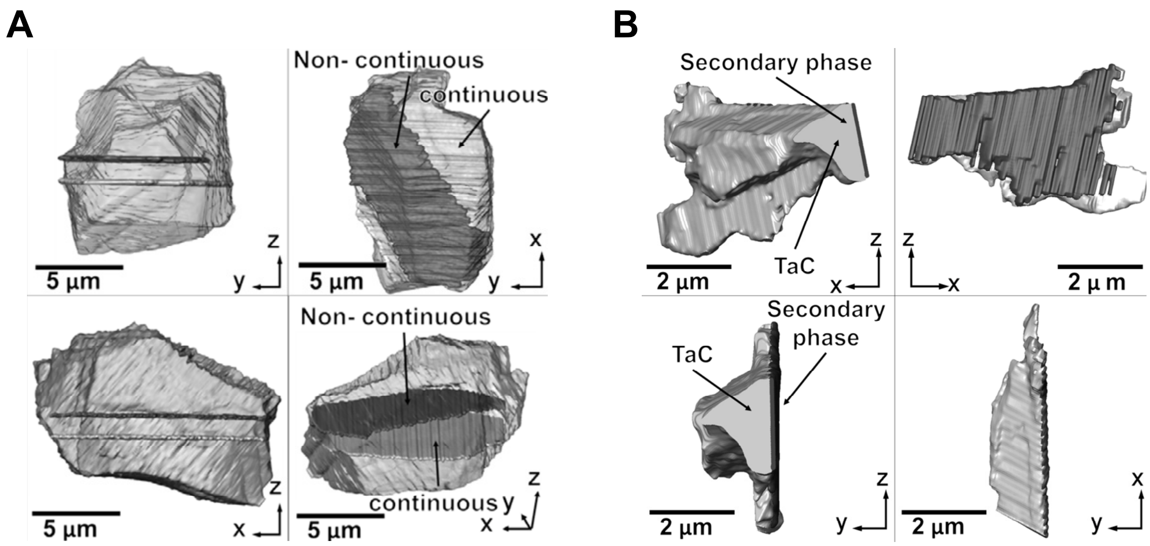

FIGURE 5

3D Reconstructions of a grain in $Ta_{55}C_{45}$ and $Ta_{63}C_{37}$. (**A**) The reconstruction of $Ta_{55}C_{45}$ shows the grain contained two types of laths; one continuous though the entire grain and one lath that terminated in the middle of the grain, labeled non-continuous. (**B**) The reconstruction of $Ta_{63}C_{37}$ shows the grain contained a thickened secondary phase spanning the entire grain; the ribbed surface of the grain is an artifact of the 3D reconstruction.

Based on this improved understanding of the thermomechanical behavior of tantalum carbides, long-term applications for the Army include rocket nozzle and other high operating temperature applications based on reduced fabrication costs and efficiencies.

F. Nanoscale Deformation and Toughening Mechanisms of Nacre Revealed

Professor Xiaodong (Chris) Li, University of South Carolina, Single Investigator Award

Nacre, also known as mother of pearl, is a natural nanocomposite composed of 95% aragonite (calcium carbonate) lamella and 5% organic biopolymer matrix, yet it is two-times stronger and 1000x tougher than the constituent materials. In this project, the investigators are using atomic force microscopy (AFM) during three-

point bend to probe the unknown role of the biopolymer matrix in the strengthening and toughening of nacre, and to determine how the biopolymer behaves during mechanical deformation (see FIGURE 6).

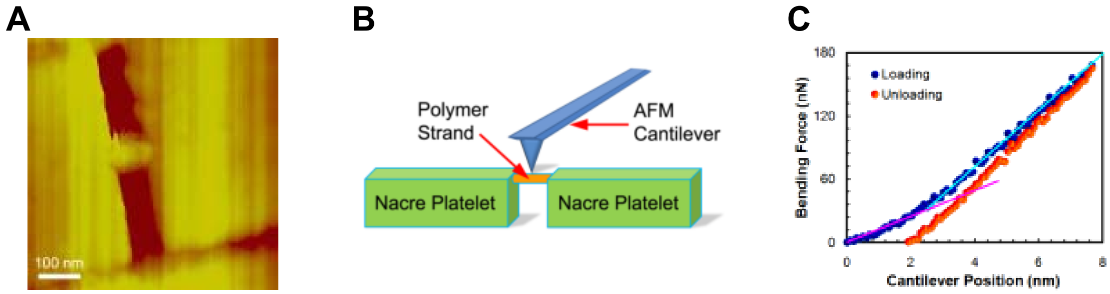

FIGURE 6

AFM bending test of biopolymer strand. The figure includes (**A**) an AFM image of a single 100 nm x 36 nm diameter biopolymer strand stretching between aragonite platelets, (**B**) a schematic of the setup of AFM bending test, and (**C**) a typical bending force-cantilever position curve of bending test.

The investigators discovered that the biopolymer matrix in nacre has the capability to strengthen itself during deformation. A spring model is proposed to explain the deformation toughening mechanism. It is believed that the deformation toughening mechanism of biopolymer matrix contributes to the extraordinary toughness of nacre together with other toughening mechanisms such as, crack deflection, deformability of aragonite platelets, aragonite platelet slip, interlocks from platelet surface nanoasperities, and rotation and deformation of nanoparticles. These new findings establish a constitutive foundation for modeling of the deformation behavior of nacre with broad long-term applications in toughened nanocomposite structural materials and protective systems.

G. Time Bunching Effect of Conformational Dynamics in Enzymatic Reactions

Professor H. Peter Lu, Bowling Green State University, Single Investigator Award

The objective of this research effort is to use mechanical and optical control of single-molecule protein conformations to explore unprecedented properties and capture exclusive states in real-time with extraordinary molecular sensitivity. The work incorporates the use of AFM to pull and hold a specific residue site of proteins, single-molecule fluorescence resonant energy transfer (FRET) imaging and single-molecule activity assays to probe protein conformations and the associated activities, and ultrafast laser photochemical cross-linking and photochemical affinity labeling to capture and mark the transient conformations.

Molecular conformational motions are generally considered stochastic phenomena. The research team has recently identified an unprecedented bunching effect associated with substrate-enzyme complex formation in T4 lysozyme conformational dynamics under enzymatic reactions. This observation indicates that conformational motion times bunch in a finite and narrow time window resulting in non-random molecular conformational motions. More specifically, the bunching effect suggests that certain enzymatic conformational motion times in forming the enzyme-substrate ES* state tend to be distributed in a finite and narrow time window measured by our single-molecule spectroscopy experiments. It is likely that the substrate binding selectively shifted the equilibrium among the fluctuating conformations of the enzyme which energetically and dynamically regulated the hinge-bending motions into a specific conformational fluctuation time range. The research has also shown that a non-equilibrium rate process through a sequence of consecutive Poisson processes with comparable rates ultimately produces a bunching effect within the overall multiple-step rate process. The characteristics of the non-equilibrium conformational fluctuation dynamics have been experimentally observed by oscillatory fluctuations of the conformational motions and Gaussian-like formation time distributions.

The conformational dynamics are significantly regulated by the interactions between the T4 lysozyme and the substrate in terms of electrostatic attraction and hydrogen bonding interactions as they are associated with the formation of the active complex state of ES* for the T4 lysozyme enzymatic reactions (see Figure 7). Based on this first-ever observation of a bunching effect in enzymatic reactions, long-term applications for the Army are anticipated in terms of robust protein folding and enzyme design for revolutionary transport, sensing, and decontamination applications.

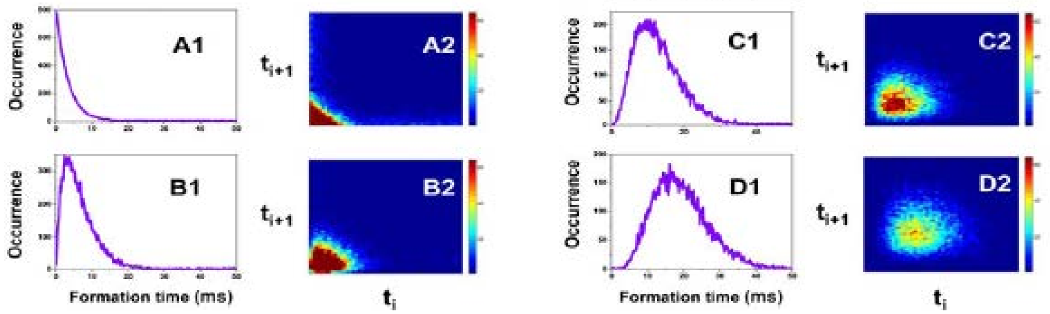

FIGURE 7

Simulated distribution of formation times and 2D joint probability distributions of adjacent formation times for different intermediate steps. Formation times (**A1-D1**) and corresponding probability distributions (**A2-D2**) are indicated in the figure. As a single step, A1 shows exponential distribution and A2 only shows a wing structure implying one step is a Poisson process and there is no bunching effect. However, for multiple steps such as 2, 4, 6 steps, nonexponential distributions of the probabilities (in B1, C1 and D1) and the bunching structures (in B2, C2 and D2) are increasingly clear, implying a bunching nature in conformational motion times.

H. Creep Far Below T_g in Bulk Metallic Glasses

Professor Yue Wu, University of North Carolina, Chapel Hill, Single Investigator Award

This goal of this project is to utilize nuclear magnetic resonance (NMR) characterization of microalloying-induced structural changes to investigate local structures and dynamics of bulk metallic glasses and the composition dependence of glass forming ability. Since diffraction approaches are insensitive to details of amorphous structures such as bulk metallic glasses (BMGs), and traditional light scattering and dielectric approaches cannot be applied to metallic systems, NMR is a uniquely valuable tool for studying metallic supercooled liquids and glasses. In addition since functional properties of BMGs, such as plasticity, have also found to depend sensitively on composition, potential correlation of functional properties with local structures, structural heterogeneity, and electronic properties are also being studied. One of the great challenges in the study of BMGs is to gain a fundamental understanding of deformation mechanisms since dislocations are absent in amorphous systems. In recent years, the focus of experiments has been on inhomogeneous deformation occurring at shear bands formed under stress above the yield strength. Many theoretical discussions have focused extensively on the fundamental issue of homogeneous deformation in BMGs such as the idea of shear-transformation-zone (STZ); therefore, this project is identifying the structural changes that occur under the operation of STZs at various stages of mechanical deformation. The results of the analysis of $La_{50}Ni_{15}Al_{35}$ BMG are shown in FIGURE 8.

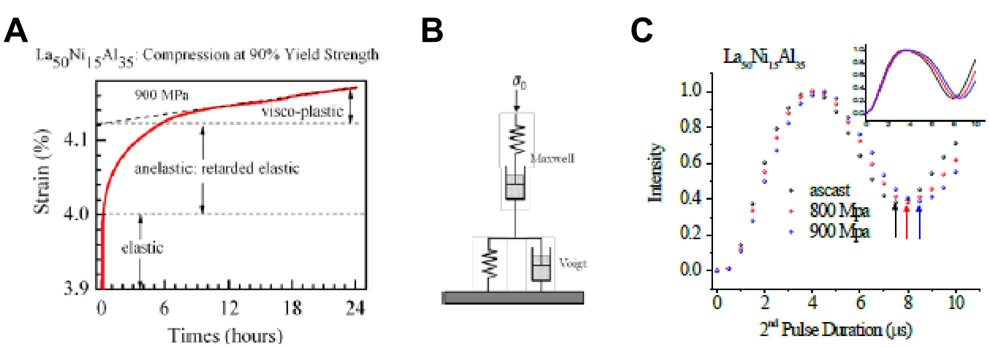

FIGURE 8

Analysis of $La_{50}Ni_{15}Al_{35}$. (**A**) Room temperature creep curve of $La_{50}Ni_{15}Al_{35}$ BMG under compressive stress at the 90% level of the yield strength, (**B**) a model of visco-elastic-plastic deformation, and (**C**) a ^{27}Al NMR nutation experiment of $La_{50}Ni_{15}Al_{35}$ BMG reveal that clear changes are observed when samples are preloaded for 24 hrs with compressive stress of 800 Mpa (80% yield strength) and of 900 Mpa (90% yield strength). The Al site symmetry increases after preloading.

The room temperature creep curve of $La_{50}Ni1_5Al_{35}$ BMG under a compressive stress of 900 MPa is shown in FIGURE 8A. As this is at the level of 90% of the yield strength (1.0 Gpa), the change is homogeneous with no shear band formation. Three modes of deformation were observed: (i) the instantaneous elastic deformation, (ii) the anelastic deformation with delayed response, and (iii) the visco-plastic deformation. FIGURE 8B shows the viscoelastic-plastic model based on springs and dashpots that reproduce the behavior in FIGURE 8A. Very recently, this research has demonstrated that local symmetry (or deviations from spherical symmetry) is a sensitive order parameter of local structures and such symmetry depends sensitively on the state of the glassy structure. Specifically the research has demonstrated that minor addition of element, even at 0.2% level, could lead to significant changes of glass forming ability accompanied by noticeable changes of local symmetry. The nutation curve of ^{27}Al in $La_{50}Ni_{15}Al_{35}$ BMG is shown in FIGURE 8C. The shift in the NMR signal intensity minimum versus the nutation time is a direct consequence of the change of local symmetry. In fact, the symmetry increases after preloading for 24 hours under stress of 800 Mpa and 900 Mpa (shift to longer time means higher symmetry).

These new insights into the microscopic origins of mechanical deformation, structural relaxation, and the stability of the supercooled liquid state, are expected to have significant long-term application for the Army in the areas of lower cost, lower weight, higher ductility alloys for a range of structural and defense applications.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Multimodal Optical Scalpel

Investigator: Vasily Astratov, University of North Carolina (UNC), Charlotte, Single Investigator Award
Recipient: Wilmer Eye Institute; Applied Physics Laboratory, Johns Hopkins University

The objective of this research project is to develop new high throughput techniques for selecting groups of supermonodispersive microspheres, self organizing these into closely spaced 3D arrays, and finally investigating the mechanisms of optical coupling and wave propagation in resonant optical circuits composed of arrays of these nearly identical microresonators. Researchers at UNC-Charlotte have shown that chains of microspheres can achieve compact focusing of light from multimodal sources. The formation of these optical microjets is now being exploited in the development of novel focusing microprobes (see FIGURE 9).

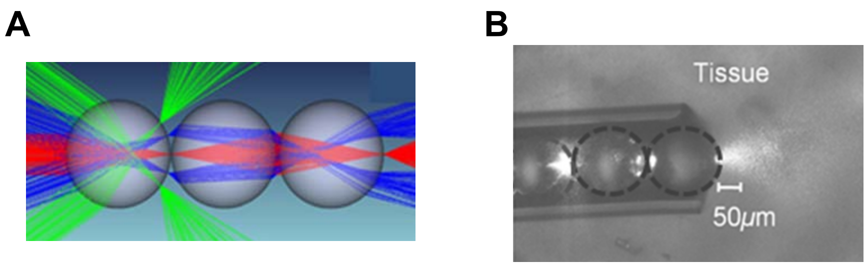

FIGURE 9

Optical microjets and scapel. (**A**) Ray tracing shows the formation of an optical microjet, and (**B**) a micrograph reveals an actual optical scalpel.

By assembling chains of the spheres inside micro-capillaries or hollow waveguides the focusing optics can easily be integrated with medical lasers to produce flexible delivery systems that can be used for a variety of biomedical applications. The system is particularly attractive due to the fact that the beam is periodically focused down to progressively smaller sizes as it passes along the chain, and the optics provide broad spectral transmission properties with high coupling efficiency and small propagation losses on the order of 0.1 dB/sphere. The researchers have found that by using high-index spheres, these chain structures can focus light into tissue in a "contact mode" that provides strong laser-scalpel interaction with the tissue that is in close proximity to the end sphere. This technology is now being investigated for possible commercialization as a novel contact laser-scalpel for ophthalmic surgeries. Collaborative research directed at using these novel scalpels in retinal surgery has been started with Professor Howard Ying, an assistant professor of ophthalmology in the Wilmer Eye Institute and Applied Physics Laboratory at Johns Hopkins University. Similar collaborative efforts are also underway with Professor Andrew Antoszyk, a vitreo-retinal surgeon at Charlotte Eye Ear Nose and Throat Associates. Finally, ex-vivo testing of these scalpels is being performed using infrared medical lasers in collaboration with Professor Nathaniel Fried's biomedical optics group at UNC-Charlotte.

B. Materials Design through New Chemical Precursors

Investigator: Charles Winter, Wayne State University, Single Investigator Award
Recipient: Sigma-Aldrich Corp. SAFC Hitech

The goal of this research effort is to synthesize novel strontium, barium, and lanthanide precursors with high thermal decomposition temperatures, while maintaining acceptable volatility for use in chemical vapor deposition (CVD) and atomic layer deposition (ALD) film growth processes. The materials of interest in this project include $SrTiO_3$, $BaTiO_3$, $Sr_xBa_{1-x}TiO_3$, lanthanide-doped group III-V semiconductors, and lanthanide oxides etc. Thermally stable Sr and Ba precursors with thermal decomposition >400 ºC for Sr and ~380 ºC for

Ba are prepared through conducting systematic investigations on different ligands that promote high thermal stability, good volatility, and appropriate reactivity toward oxygen sources in strontium, barium, and lanthanide precursors. It was discovered that for Sr and Ba, tris(pyrazolyl)borate (Tp) ligands and derivatives with alkyl substituents in the 3- and 5-positions of the pyrazolyl groups, can combine monomeric structures with high volatility and exceptionally high solid state decomposition temperatures (see FIGURE 10). Using these precursors and water as the oxygen source, very high temperature self-limited growth (ALD growth at up to 400 ºC) of metal borate films of the composition MB_2O_4 (M = Ca, Sr, Ba) was demonstrated.

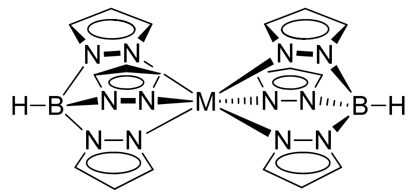

FIGURE 10

Core structure of group 2 Tp complexes

Professor Winter has initiated a collaboration with ARL scientists engaged in thin film growth of ferroelectrics ($Sr_xBa_{1-x}TiO_3$ growth) for the selection of appropriate precursors. In addition, the precursors $CaTp_2$, $SrTp_2$, and $BaTp^{Et2}_2$ developed in this project are being commercialized by SAFC Hitech, Haverhill, MA. Professor Winter has submitted a U.S. patent application on a class of ligands that impart high thermal stability to metal complexes. These novel precursors are essential to make high quality ferroelectric and piezoelectric crystalline films that are being used in Army applications in nonvolatile memories, buffer layers, integrated optics, photonics, smart materials, and solid state near infrared lasers.

C. Lattice Engineering for Novel Materials and Devices

Investigator: Eugene Fitzgerald, Massachusetts Institute of Technology, Single Investigator Award
Recipient: 4Power LLC

The objective of this research is to explore lattice-mismatched semiconductor materials and lattice-matched heterovalent interfaces between the lattice constants of Si(or GaP) and Ge (or GaAs). The heterovalent interface of GaAsP/SiGe is of interest due to the applications in high efficiency solar cells and other applications. The reason for this interest is that SiGe-GaAsP-InGaP lattice-matched triple junction cells have the optimal band-gaps for creating very high efficiency solar cells, a theoretical maximum for these band gaps of approximately 50%. Due to the investigator’s prior research in relaxed SiGe alloys on silicon (a prior project within the ARO Core Research Program), these cells can also be manufactured in a silicon manufacturing facility, resulting in lower cost than incumbent and less efficient cells. Professor Fitzgerald and his collaborator Professor Steven Ringel at Ohio State University (an investigator previously supported through ARO) co-founded 4Power LLC to commercialize this technology, and the cells based on the GaAsP/SiGe interface research have transitioned to this company. These future high efficiency lower-cost solar cells have applications in various military applications, including remote power for charging Soldier equipment as well as solar-powered UAV’s. 4Power LLC has received American Recovery and Reinvestment Act funding for continued development of these cells.

D. High Resolution Electron Back-Scatter Diffraction

Investigator: Brent Adams, Brigham Young University, Single Investigator Award
Recipient: TSL-EDAX, Inc.

The goal of this project is to develop a suitable high resolution orientation imaging microscopy (HROIM) and demonstrate its viability and effectiveness. The research was enabled by a unique capability to provide rapid analysis of Electron Back-Scatter Diffraction (EBSD) patterns, based on the cross-correlation of EBSD patterns to recover lattice orientation and disorientation with high angular resolution (0.0050). This refined angular precision also enables recovery of the full local elastic strain field tensor, to a precision of 10-4. The research has now resulted in code that will be incorporated in a new product and it has received significant testing by TSL-EDAX. Additionally, TSL-EDAX results demonstrated an order of magnitude improvement in angular resolution. Further work is now underway to improve pattern center placement to achieve improved results.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Spin Injection Currents using the Spin Hall Effect (SHE)

Professor Dan Ralph, Cornell University

Researchers at Cornell University discovered that a substantial spin current can be generated by the flow of a longitudinal electrical current in a thin Pt layer, due to its large spin orbit scattering probability. The magnitude of the spin current was quantified by measuring its effect on an adjacent permalloy (magnetic) layer. When an in-plane RF current was generated in the Pt layer it induced an oscillating transverse spin current that exerted an oscillating spin torque on the adjoining permalloy layer. This oscillating torque induced a precession of the permalloy moment and generated a measurable resonant response in the permalloy layer when the frequency and DC bias magnetic field satisfied the FMR resonance condition. Experimentally the in-plane DC field was applied at a 45 degree- angle to the direction of current to enable detection of the precession via the anisotropic magnetoresistance effect. This effect resulted in a significant oscillation of the permalloy resistance that mixed with the original rf current to produce a DC voltage across the sample. This DC voltage provided a direct measure of the magnitude of the spin current, which proved to be about 5% of the original longitudinal current flow. This discovery represents a new alternative approach for injecting pure spin currents into device structures. Initial estimates indicate that the spin current density injected into a semiconductor using this SHE generated transverse spin current will likely be much higher than that which is currently achieved with polarized current injection through Schottky or insulating tunneling barriers. It is anticipated that in the coming year the researchers will determine whether the required ohmic contacts can be formed in a manner that avoids substantial spin-flip scattering within the contact region.

B. Thermodynamic Stabilization of Powder Route Nanocrystalline Tungsten Alloys

Professor Christopher Schuh, Massachusetts Institute of Technology

The goal of the project led by Professor Schuh's research group is to develop a tungsten-rich alloy powder that can be produced readily in a nanocrystalline form that is sufficiently stable to resist significant structural change during high-temperature consolidation to full density. To achieve this goal, the researchers employ both theoretical modeling, to identify candidate alloys with improved stability in the nanocrystalline state, and experimentation, to produce and test alloy powders and validate the model.

It is anticipated that using a systematic modeling effort, the PI will identify alloying strategies that can stabilize a nanoscale grain structure. Specifically alloying can stabilize nanocrystalline structures through either grain boundary segregation or the precipitation of intermetallic phases in the intergranular region. Previous work by Professor Schuh's group led to the development of a general thermodynamic model for the free energy of mixing in binary alloys in which the tendency for grain boundary segregation of a solute can be compared between material systems. A few material specific parameters are required, such as pair-wise interactions, atomic volume, and grain boundary energy, but given these the model can then predict trends in segregation behavior. A minimum in the free energy can be found with respect to the grain size and concentration of solute segregated to the grain boundary for a global solute concentration. The model thus directly provides insight on how an alloying element can stabilize a nanocrystalline structure. Using this model, it is anticipated that the investigator will identify a suitable alloying element to refine the grain size of tungsten. The discovery of a methodology to produce stable full-density nanocrystalline tungsten could have significant potential in kinetic energy penetrator applications where a high-density and self-sharpening via shear localization are critical top optimal performance.

C. Synthesis and Properties of Mono- and Few-layer Hexagonal Boron Nitride (h-BN) Films

Professor Rodney Ruoff, University of Texas at Austin

The goal of this research is to synthesize crystalline 2D free standing films and to characterize these materials for unique optical, electronic, thermal, mechanical and surface properties. The effort utilizes chemical vapor deposition to grow free standing monolayer films on metallic substrates and incorporates a variety of different precursors to systematically explore different experimental variables, such as time-temperature profile, pressure, flow rate, substrate composition, and gas mixture composition to obtain optimal films. The research group will perform experiments to investigate nucleation and growth mechanisms of free standing monolayer or a few-layer 2D h-BN films on metallic substrates (*e.g.*, Cu- Ni alloys). The investigator plans to construct a chemical vapor deposition reactor and systematically explore different experimental conditions such as time- temperature profiles, pressure, flow rate, substrates, gas mixtures etc., to develop the necessary understanding of processing-structure-property relationships of 2D h-BN films. All these factors are expected to influence the chemical composition, defect density, thickness, etc., and hence the final properties of the films. It is anticipated that the results of this study will enable the processing of 2D h-BN films with exceptional properties. Free standing 2D h-BN films complement 2D graphene films that are being developed for a variety of DoD applications. These films could potentially lead to future high frequency, low power RF applications, flexible electronics, nano-electromechanical (NEMS) systems as well as deep UV light-emitting devices.

D. Predicting Shape-dependent Pattern Formation in Belousov-Zhabotinsky (BZ) Gels

Professor Anna Balazs, University of Pittsburgh

Researchers at the University of Pittsburgh are developing novel theory and simulation to design materials that harness mechanochemical transduction to both signal the occurrence and extent of external load on a material and initiate a response. Gels exhibiting the Belousov-Zhabotinsky (BZ) reaction exhibit a distinct form of mechanochemical transduction - the application of the external forces causes a traveling chemical wave to spread through the material. This behavior is sensitive to both the magnitude of the force and the period of time that the force is applied. The goal of this research effort is to experimentally validate predicted shape-dependent pattern formation resulting from the periodic reduction and oxidation of the Belousov-Zhabotinsky (BZ) catalyst. Computational models of these BZ gels have predicted that oscillating patterns can be modulated by changing the physical shape and size of such gels.

Research will resolve the effects of gel aspect ratio and absolute dimensions for both covalently bound and physically associated catalysts. It is anticipated that the research team will identify the factors governing pattern formation at both early and late reaction times, and the gel durability requirements for undergoing these reactions without significant degradation or perturbation in pattern formation will be determined. This research is expected to contribute to long-term Army interests in advanced coatings, propellants, and permselective polymeric materials.

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CHAPTER 9: MATHEMATICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Mathematical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research efforts to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. The results of these research efforts will stimulate future studies and help to stay the U.S. at the forefront of research in the mathematical sciences.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of mathematical concepts, structures, and algorithms, the research efforts managed in the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research may provide protection against future biological and chemical warfare agents, improve wound-healing, lead to self-healing communication networks, enhance cognitive capabilities for the Soldier, and contain or prevent infectious disease. The results may provide full (*i.e.*, not only physical) situational awareness through multi-target recognition/tracking/monitoring of physical, informational, cognitive and social targets in asymmetric, often urban scenarios. It may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy. It may also provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, and may enable next generation communication networks along with improving weapon design, testing, and evaluation.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. The Mathematical Sciences Division coordinates efforts with the Network Sciences Division to pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division also coordinates efforts with the Physics Division to pursue fundamental research on quantum control. Research efforts also complement initiatives in the Life Sciences Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better

understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. Mathematical Sciences programs interface with the Engineering Sciences Directorate Program Areas on understanding the mechanics of fluids in flight and understanding combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Mathematical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Numerical Analysis. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army, by identifying yet unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered if the phenomena are so complex that such frameworks are not feasible. The identification of accurate metrics is part of the mathematical framework and is of great interest, as traditional metrics often do not measure the characteristics in which observers in general, and the Army in particular, are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. This Program Area is divided into three research Thrusts: (i) Information Fusion in Complex (physical, informational and social) Networks, (ii) Geometric and Topological Modeling of Irregular Objects and Functions and (iii) Analytical Foundations for Human Cognitive, Behavioral and Social Modeling.

Research progress on improved information fusion in distributed sensor networks, including and especially hard/soft (all-source) fusion networks ("hard" = physics-based, "soft" = human-based), will ultimately fulfill Army C4ISR requirements for tractable/scalable methods for identification and tracking of hard and soft targets (physical, informational, cognitive, social). Mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km is important for situational awareness, mission planning and training. In addition, mathematical analysis for human cognitive, behavioral and social modeling is important for identifying "soft targets" (human beings, social networks, intentions) in asymmetric defense.

2. Probability and Statistics. The goal of this Program Area is to create innovative theory and techniques in stochastic/statistical analysis and control. Basic research in probability and statistics will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare. This Program Area is divided into two Thrust areas: (i) Stochastic Analysis and Control, and (ii) Statistical Analysis and Methods.

The goal of the Stochastic Analysis and Control Thrust is to create the theoretical foundation for modeling, analysis, and control of stochastic networks and stochastic fluid turbulence. Many Army research and development programs are directed toward modeling, analysis, and control of stochastic dynamical systems. Such problems generate a need for research in stochastic processes, random fields, and/or stochastic differential equations in finite or infinite dimensions. These systems often have non-Markovian behavior with memory for which the existing stochastic analytic and control techniques are not applicable. The research topics in this Thrust include, but are not limited to, the following: (i) analysis and control of stochastic delay and partial differential equations; (ii) complex and multi-scale networks; (iii) spatial-temporal event pattern analysis; (iv) quantum stochastics and quantum control; (v) stochastic pursuit-evasion differential games with multi-players; and (vi) other areas that require stochastic analytical tools.

The objective of the Statistical Analysis and Methods Thrust is to create innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. The research in this Thrust supports the Army's need for real-time decision making under

uncertainty and for the design, testing and evaluation of systems in development. The following research topics are of interest to the Army and are important in providing solutions to Army problems: (i) Analysis of very large or very small data sets, (ii) reliability and survivability, (iii) data, text, and image mining, (iv) statistical learning, (v) data streams, and (vi) Bayesian and non-parametric statistics.

Potential long-term applications for research carried out within this Program Area include optimized design and operation of robust and scalable next-generation mobile communication networks for future network-centric operations made possible through advances in stochastic network theory and techniques. Also, advances in stochastic fluid turbulence and stochastic control of aerodynamics can improve the maneuvering of helicopters in adverse conditions and enable optimal design of supersonic projectiles. In addition, new results in density estimation of social interactions/networks will help detect adversarial behaviors and advances in spatial-temporal event pattern recognition and will enable mathematical modeling and analysis of human hidden intention and will provide innovative approach for counter-terrorism and information assurance. Finally, new discoveries in signature theory will significantly improve reliability of Army/DoD systems and experimental design theory, and will lead to accurate prediction and fast computation for complex weapons.

3. Biomathematics. The goal of this Program Area is to identify and mathematize the fundamental principles of biological structure, function and development across biological systems and scales. The studies in this program may enable revolutionary advances in Soldier health, performance, and materiel, either directly or through bio-inspired methods. This Program Area is divided into three research Thrusts: (i) Modeling, Analysis, and Control of Biological Systems, (ii) Computational Biology, and (iii) Fundamental Laws of Biology. Within these Thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Research in the Modeling, Analysis, and Control of Biological Systems Thrust area focuses on finding realistic, yet mathematically tractable, mechanistic models for a variety of biological networks, both static and dynamic, along with methods for their control. Efforts in the Computational Biology Thrust area seek to elucidate and model the fundamental principles by which biological elements such as genes, proteins, and cells are integrated and function as systems. Research in the Fundamental Laws of Biology Thrust area is high-risk research in biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research efforts in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Numerical Analysis. The goal of this Program Area is to develop a new mathematical understanding to enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The studies guided by this program may enable the algorithmic analysis of current and future classes of problems by identifying yet-unknown basic computational principles, structures, and metrics, giving the Army improved capabilities and capabilities not yet imagined in areas such as high fidelity modeling, real-time decision and control, communications, and intelligence. This Program Area is divided into three research Thrusts: (i) Multiscale Methods, (ii) PDE-Based Methods, and (iii) Computational Linguistics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. The goal of research in the Multiscale Methods Thrust is to achieve higher fidelity and more efficient modeling of multiscale phenomena in a variety of media, and to create general methods that make multiscale modeling accessible to general users. Efforts in the PDE-Based Methods Thrust focus on establishing the mathematics required for higher fidelity and more efficient modeling of sharp-interface phenomena in a variety of media, to discover new methods for coefficient inverse problems that converge globally, and to create reduced order methods that will achieve sufficiently-accurate yet much more efficient PDE solutions. Efforts in the Computational Linguistics Thrust focus on creating a new understanding of natural language communication and translation through new concepts in structured modeling.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include force protection concrete and improved armor, more stable but efficient designer munitions, high density, rapid electronics at low power, and nondestructive testing of materials. Program efforts could also lead to more capable and robust aerial delivery systems, more efficient rotor designs, systems to locate explosive ingredients, more efficient combustion designs, and real-time models for decision-making. Finally, efforts within this program may lead to natural language interactions between bots and humans in cooperative teams, new capabilities for on-the-ground translation between deployed U.S. forces and locals, especially in low density language regions, new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

C. Research Investment

The total funds managed by the ARO Mathematical Sciences Division for FY10 were $19.2 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $3.3 million. The DoD Multidisciplinary University Research Initiative (MURI) and Defense University Research Instrumentation Program (DURIP) provided $14.8 million to programs managed by the Mathematical Sciences Division. The Division also managed $0.6 million of Defense Advanced Research Projects Agency (DARPA) programs. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $0.9 million for awards in FY10. Finally, $0.1 million in FY10 was provided for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) outreach program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Remote Detection of Covert Tactical Adversarial Intent of Individuals in Asymmetric Operations (Adelphi, MD; 7-8 December 2009). The goal of this workshop was to design a first-order road map for research to bridge the scientific gap between observations from physical sensor networks at 3–50 meters and determination of covert tactical adversarial intent of individuals. The workshop had both plenary sessions/discussion and break-out sessions for three working groups (cognitive/perceptual phenomena, sensors, and information fusion). The results of the workshop were reported in the 28-page ARL Special Report ARL-SR-197 and an eight-page summary of the report presented under the title "Remote Detection of Covert Tactical Adversarial Intent of Individuals in Asymmetric Operations" at the 13th International Conference on Information Fusion (July 2010). The workshop affirmed that remote detection of covert tactical adversarial intent of individuals in asymmetric operations is an area that is feasible and holds great promise for the future. Participants in this workshop included the ARO Mathematical Sciences Division, ARL's Computational and Information Sciences Directorate (ARL-CISD), ARL's Human Research and Engineering Directorate (ARL-HRED), ARL's Sensors and Electron Devices Directorate (ARL-SEDD), the U.S. Army's Communications and Electronics Command's (CECOM's) Night Vision and Electronic Sensors Directorate (NVESD) and Intelligence and Information Warfare Directorate (I2WD), the U.S. Air Force Research Laboratory's (AFRL's) Human Effectiveness Directorate, and the Defense Academy for Credibility Assessment (DACA).

2. International Conference on Information Fusion 2010 (Edinburgh, UK; 26-29 July 2010). This annual conference, organized by the International Society for Information Fusion (ISIF) and administered by the UK's Institution of Engineering and Technology (IET), brought together professionals from around the world to facilitate discussion on the recent advances and pertinent issues in fusion technologies. The conference's technical scope spans methodologies, algorithmic domains, solution paradigms, sensor specific processing and fusion, and applications. Along with the conference chair, the ARO Mathematical Sciences Division organized and co-chaired the plenary session entitled "Uncertainty Forum", which investigated the representation of uncertainty in information fusion, especially hard/soft information fusion, as a central theme of the conference. ARO also organized and chaired the special session "*Object Recognition and Tracking: From Physical to Non-physical in both Target Type and Sensing Mode*", which included presentations by the ARL-ARO Urban Target Recognition MURI, the ARL-ARO Abductive Inference MURI, I2WD and a joint paper (presented by ARO) by ARL- HRED, ARL-CISD, ARL-SEDD, I2WD, NVESD, AFRL and the Defense Academy for Credibility Assessment (DACA) on detecting adversarial intent. In addition, the Mathematical Sciences Division's

Network-based Hard/soft Information Fusion MURI faculty organized and chaired the session "*Multidisciplinary Research in Hard and Soft Information Fusion*."

3. Army Conference on Applied Statistics (Tempe, AZ; 21-23 October, 2009). The goal of this conference was to provide a forum for the presentation and discussion of theoretical and applied papers related to the use of probability and statistics in solving defense problems. The conference provided an invaluable opportunity for interaction among academic, industry, and defense scientists. It also served a nurturing role in the elevation of statistical competence among defense researchers in other disciplines who find themselves statistical practitioners because of the compelling benefits statistical science brings to defense research, development, and testing. The conference was structured to include general sessions that included invited presentations on emerging topics in statistics, and special sessions that focused attention on Army problem areas for which the role of statistical science should be more fully explored. Contributions to the conference sessions included papers ranging from new methodology to interesting statistical applications. In the clinical sessions, a distinct feature of the conference, presenters sought guidance from a panel of experts on problems that have not been completely or satisfactorily solved. Other noteworthy events include a tutorial was presented on a statistical topic of interest for defense applications (presented prior to the conference). It is noted that the Army Wilks award is given periodically at this conference to an individual who has made significant contributions to the practice of statistical science in the Army through research in statistics and application of statistics in the solution of Army problems.

4. The Sixth Symposium on the Frontier of Statistical, Mathematical and Computational Sciences (Washington DC; 1-2 September, 2010). The goal of this symposium was to provide a forum for presentations and discussion on the frontiers of mathematical sciences. This symposium has a general theme of consensus, cooperation, and competition in networked multi-agent systems, with emphasis on large-scale decision-making in dynamic and uncertain environments. Special focus is placed on the theory of games, optimization, learning, and adaptation. Some common qualitative/quantitative issues are addressed, including but not limited to reliability, resilience, risk mitigation/tolerance, stability, and coherence in complex multi-agent interactive dynamical systems. The Mathematical Sciences Division partially funded and played a scientific advisory role in this symposium.

5. Computational Biology Training and Workshop (Berkeley, CA; 9-12 August 2010). The goal of this joint Life Sciences and Mathematical Sciences Division sponsored Training and Workshop was to introduce computational biology to DoD researchers and to discuss new needs in the fundamental research area of computational biology. Advances in biotechnology such as genome sequencing, proteomics, metabolomics and transcriptomics have led to an explosion of data characterizing biological systems. As the amount of such information grows exponentially, novel methods of data analysis and data interpretation are needed in order to optimally exploit this rich data collection. The two day "Crash Course in Systems Biology" training familiarized primarily biological researchers with current computational biology software and capabilities, with an emphasis on quantitative applications for understanding and modeling complex biological systems. The subsequent two day workshop brought together leaders in the field from academic and government laboratories to present the state-of-the-art in three areas: (i) experimental inference of growth requirements and interactions of environmental microbes *in situ*, (ii) enrichment and analysis of environmental microbes for laboratory study, and (iii) computational prediction of growth conditions and composition. The workshop presentations were followed by a discussion of the fundamental research needed to revolutionize our ability to perform efficient microbial data integration and, eventually, lead to an automated data processing system capable of microbial forensics analyses, among other applications of Army interest.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Mathematical Sciences Division; therefore, all of the division's active MURIs are described in this section.

1. Designing and Validating Theories of Distributed Signal Processing. This MURI began in FY06 and was awarded to a team led by Professor Shankar Sastry of the University of California, Berkeley. The goals of this research are to: (i) develop new theories of distributed signal processing with random spatio-temporal sampling of complex scenes for recognition and tracking of object in heterogeneous sensor networks (HSNs), (i) develop theories for robust design principles for sensor networks with both low- and high-bandwidth sensors to automatically recognize and track targets in complex urban environments, (iii) develop theories for metrics for the design and deployment of sensor webs, and theoretical bounds on the performance of different kinds of sensor webs and (iv) develop theories for incorporation of mobility into sensor web models and into the algorithms for these webs.

The MURI team has developed a new approach to distributed fusion in graphical models that highlights the role of key nodes. This method makes use of the notion of a feedback vertex set, i.e., a set of nodes that, if removed, render a graph cycle-free. With such a set identified, a new messaging algorithm results in which several message streams are created, culminating in fusion at the feedback vertex nodes and subsequent messaging to disseminate information throughout the graph. This algorithm provides exact answers for Gaussian inference but is computationally tractable only for graphs with modest-sized feedback vertex sets. The team has developed a method for choosing a set of most important vertices (*i.e.*, vertices that are the most significant information hubs for the graph) and then employing the same algorithm now using only these important hub vertices. The resulting algorithm yields approximate answers (since not all loops in the graph have been broken), but the results demonstrate that excellent and scalable performance is readily achieved using only modest-sized sets of hub vertices, including for graphical models for which previously developed algorithms fail to converge. The team has designed level-set methods for discrimination in both centralized and networked systems. These methods use available training data both to identify lower-dimensional projections of the data of most significance for the discrimination task and to determine decision boundaries in these reduced-dimension spaces via curve evolution. The team is currently upgrading the design of a wireless smart camera architecture that was designed in the first two years of this project. This research responds to the Army need for improved urban target recognition capabilities for military operations and for monitoring of military or terrorist activity.

2. Discovering Mathematical Theories in Spatial-temporal Nonlinear Filtering. This MURI began in FY06 and was awarded to a team led by Professor Boris Rozovsky at University of Southern California; however, Professor Rozovsky transferred to Brown University in FY07 and continued as the principal investigator (PI) of this project. The objective of this research is to invent new mathematical theory and techniques in spatial-temporal nonlinear filtering (NLF) and change-point detection (CPD) in order to develop a mathematical and systematic foundation and algorithms for spatial-temporal statistical inference and for fusion of heterogeneous information from multi-source, multi-sensor distributed sensor networks.

This research will explore three central scientific problems: (i) nonstationarity, (ii) integrating metric and symbolic information, and (iii) very high dimensionality. Current methods for pattern recognition in monitoring and surveillance, including network monitoring, are designed for stationary patterns, and cannot cope with new patterns in ever-changing environments. This project will develop new statistical methods for the nonstationarity problem, particularly spatial-temporal NLF, CPD, and advanced fusion methods. A distinctive feature of its approach is that the spaces in which estimation, classification and tracking are performed are both metric and symbolic. Just as a moving vehicle may be tracked in a metric coordinate space by conventional filters, so can an unfolding terrorist plan be tracked in plan space by a hybrid metric-symbolic nonlinear filter. To the extent that information in these spaces is dependent, each space can compensate for incomplete and ambiguous data in the other, improving fusion performance. The modern battlespace produces unmanageable amounts of data, as do the Maritime Domain Awareness and the Global War on Terror. Dimensionality, or the sheer number of objects about which information is available, grows faster than the human ability to track, fuse, interpret, and base decisions on the information. This project adapts and develops methods for quickly extracting *actionable* information, framing it for automated decision-making, and in this way helps to realize the potential of measurement and signature intelligence (MASINT), ground moving target indicator (GMTI) technology, video surveillance schemes and other massive and extremely expensive data collection programs.

3. Theories of Dynamic Modeling of 3D Urban Terrain. This MURI began in FY07 and was awarded to a team led by Professor Andrew Kurdila of the University of South Carolina. The goal of this research is to develop theory, algorithms, software, and experiments for the synthesis of urban terrain maps using dynamic point cloud sensor data. More specifically, the objective of this research is to develop theories (i) for capturing

high-order topology through implicit representation of surfaces, (ii) for developing multiscale and adaptive algorithms that enable various resolutions of the rendered surface governed by the local density of the point clouds, (iii) for the fast computation of signed distances to the terrain surface thereby giving field of view from specified observation points, (iv) for the use of dynamic point cloud measurements for the navigation and control of autonomous vehicles in three dimensions, and (v) for change detection from point cloud observations taken at different times.

The MURI team has already developed a novel method called Wavelet Streaming Surface Reconstruction (WSSR) for reconstructing surfaces from point cloud data using wavelet decompositions. It combines the advantages of the implicit methods and the multiscale structure of the wavelets (subdivision) methods. This enables one to extract a polygonal model of the boundary by applying an octree contouring method to create a water-tight, adaptive contour, which is guaranteed to produce a topological and geometrical manifold. One of the great advantages of this approach is its locality. Each sample influences only a small number of coefficients in the representation. The method is very general in the sense that it can use any orthogonal or biorthogonal compactly supported wavelet basis. This research responds to the Army need for 3D urban terrain models for simulation, training, mission planning, operational situational awareness and vehicle navigation.

4. Analysis and Design of Complex Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Jean Walrand of University of California, Berkeley. The goal of this research is to invent new mathematical theories and techniques that will enable modeling, analysis and control of complex multi-scale networks. These theories will ultimately enable the development of a unified framework for understanding and exploiting complex behaviors of the network resulting from spatial and temporal heterogeneity and the interaction of network algorithms with traffic characteristics.

More specifically, the objective of this MURI is to: (i) understand the interaction of traffic statistics, including long-range dependence (LRD) properties, and control actions across timescales, from back-clocking and burstiness effects at the sub-round-trip-time (sub-RTT) timescale, congestion control at RTT timescales, inter-domain routing at the time scale of minutes or hours, to revenue maximization and peering structure on the scale of days and months, (ii) design strategies for controlling admissions of new connections, flows of admitted connections, and the pricing of connections taking into account the LRD property of the traffic, (iii) develop theories for maximizing network utilization in the presence of wired and wireless links (which typically pose significant challenges for the proper utilization of network resources by end-to-end rate control protocols), and (iv) design traffic-measurement techniques in a heterogeneous environment, which can have significant implications for monitoring, management, and security of the network. The new distributed algorithms for wireless networks that may result from this work have the potential of revolutionizing *ad hoc* networks by enabling the design of simple, robust, and efficient protocols. Improved WiFi protocols increase the throughput by a significant factor and the fundamental theoretical research by this MURI team on LRD will produce new mitigation methods such as optimal fragmentation and diversity routing.

5. Discovering New Theories for Modeling and Analysis of Multi-scale Networks. This MURI began in FY08 and was awarded to a team led by Professor Ness Shroff at the Ohio State University. The objective of this research is to invent new mathematical theory and techniques in order to enable modeling, analysis and control of complex multi-scale networks. In particular, the research will develop a mathematical theory and techniques for modeling, analysis, and control of complex multi-scale networks.

The research team is investigating multi-scale phenomenon and control of wireless systems including LRD in wireless systems, which is a consequence of the temporal and spatial complexity inherent in military networks. The research focuses on the impact of multi-scale phenomena on the control, performance, and security of these networks. This research will lead to a long-overdue union of stochastic control, statistics, queuing theory, complexity theory, and the distributed algorithms, which is necessary for the development of radically new strategies for controlling the increasingly complex military networks. In particular, the objective is to develop a unifying theory that is mathematically rigorous and leads to practically-implementable network control and distributed detection algorithms, thus providing an enormous tactical advantage for the U.S. military.

The research approach consists of three inter-related focus areas: (i) traffic modeling and analysis, (ii) network control, and (iii) information assurance. While the investigation covers both wired and wireless networks, it focuses heavily on the wireless portion of the overall networks, which is central to tactical communications and the Army's network centric operations, and is likely to have the most stringent resource constraints and greatest

vulnerability to security breaches. The modeling approach takes into account the critical time scales in military networks, from user level applications (*e.g.*, time-critical data), to the time-scale required for the operations of various protocols and resource allocation schemes; this is significantly different from the state-of-the-art in traffic modeling, where the network is viewed as a physical entity whose laws are being passively observed through traffic studies. The team is formulating optimization and distributed control problems for providing network services and studies the impact of LRD traffic on network control, performance, and security. The project is also developing an integrative approach that combines the LRD modeling and network control to obtain non-parametric or semi-parametric techniques for the distributed detection of information flow and flow changes needed for preventing security attacks. The research is characterizing the ability of flow to be detected as a function of flow rate, delay and memory constraints, and develops distributed detection schemes that guarantee vanishingly low detection error probabilities. The outcomes of this project will result in distributed, low-complexity, and robust control mechanisms for achieving high network performance, intrusion detection, and security. These outcomes will provide high performance, reliability, and information assurance in support of the Army's future Network-Centric Operations and Network Centric Warfare (NCW). Further, the rigorous and conceptually unifying mathematical techniques developed in the course of this work will enable a deeper understanding of the dynamics and control of large and complex networks.

6. Network-based Hard/soft Information Fusion. This MURI began in FY09 and was awarded to a team led by Professor James Llinas of the University at Buffalo. The goals of this research are to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) Level 1 and Level 2 data fusion environment.

The MURI team is investigating source characterization of soft data input streams (human observation direct and indirect, open source inputs, linguistic framing, and text processing), common referencing and alignment of hard and soft data, generalized data association strategies and algorithms, robust estimation, dynamic network-based effects on fusion architectures, and test and evaluation. The team has already made progress in the following areas: creation of an overall system concept for human-centered information fusion and information processing architecture; development of an evolutionary test and evaluation approach that proceeds from "truthed" synthetic hard and soft data to human-in-the-loop experiments; creation of a counter-insurgency-inspired synthetic data set involving both hard and soft data; development of initial hard sensor processing algorithms for level 0-1 processing; development of a taxonomy for characterizing the human as observer (source characterization); selection of a tool for processing text messages, including semantics; development of an overall architecture and framework for soft data association that extends the traditional hypothesis generation-hypothesis evaluation-hypothesis selection paradigm for fusion of soft data and utilizes a data graph association process; development of a new method for data representation of image and acoustic data; and development of methods for representing uncertainty in soft data. This research responds to the Army need for hard/soft fusion models for operations, mission planning, training and simulation.

7. Modeling Approach for Translation. This MURI began in FY10 and was awarded to a team led by Professor Jaime Carbonell at Carnegie Mellon University. The goal of this MURI is to investigate new concepts for language translation that use structured modeling approaches rather than statistical methods.

Whereas statistical approaches for machine translation (MT) and text analysis (TA) successfully harvest the low-hanging fruit for large data-rich languages, these approaches prove insufficient for quality MT among typologically-diverse languages and, worse-yet, are inapplicable for very low-resource languages. This research is venturing much further than just introducing syntactical structures into statistical machine translation (SMT) and will turn the process on its head (*i.e.*, start with a true linguistic core and add lexical coverage and corpus-based extensions as data availability permits). This linguistic core would comprise an enriched feature representation (morphology, syntax, functional semantics), a suite of core linguistic rules that operate on these features via powerful operators (tree-to-tree transduction, adjunction, unification, etc.), and prototype MT and TA engines to evaluate their accuracy and phenomenological coverage. Contrastive linguistic analysis will identify the major translation divergences among typologically diverse languages, feeding into the MT linguistic core. Once the core is built, coverage will be broadened through additional linguist-generated rules and via Bayesian constraint learning from additional corpora and annotations as available - learning with strong linguistic priors, respecting the linguistic core, is expected to require much less data than unconstrained corpus-based statistical learning. The initial efforts will focus primarily on African languages, such as Chichewa and Kinyarwanda (both from the Bantu family), Tumak (an Afro-asiatic Chadic language), Dholuo (a Nilo-Saharan

language), and for even greater typological diversity, a Mayan language, such as Uspanteko. In addition to designing, creating, documenting and delivering the linguistic cores for the selected languages, this program focuses on delivering a suite of methods and algorithms (*e.g.*, tree-to-tree feature-rich transducers, proactive elicitors, rule interpreters) and their prototype software realizations.

The new powerful linguistic capabilities potentially generated by this research will enable the Army to perform rapid and principled construction of MT and TA systems for very diverse low-density/low-resource languages. This has the potential to provide the Army with new tactical capabilities for on-the-ground translation between deployed US forces and locals, especially in low density language regions. It also has the potential for new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

8. Modeling the Effects of Training on Performance. This MURI began in FY10 and was awarded to a team led by Professor Alice Healy of the University of Colorado - Boulder. The goal of this research is to develop an empirically-based theoretical framework that can account for and make accurate predictions about the effectiveness of different training methods for militarily relevant tasks.

The research is proceeding in three directions (i) the development and testing of training principles, (ii) the development of principles on the acquisition and retention of basic components of skill, and (iii) the theoretical and computational modelling of training effects associated with levels of automation, individual differences, and team performance. To render the study of training effects tractable and to guide research, the MURI team has developed a multi-dimensional taxonomy that provides a framework by which training effects can be assessed and predicted for any task. The taxonomy involves a four-dimensional decomposition of the training space, including separate dimensions of classification for task description, training procedure, and the context and assessment of task performance. The training principles are considered the fourth dimension. The component of the project devoted to models consists of four parts: a data entry task, a more complex radar tracking task, an information fusion task, and stimulus-response compatibility effects. The research on model assessment is focused on model optimization. The Army has a significant need for research in training and training management, and this MURI team will make contributions to meet this need by providing performance-shaping functions (*i.e.*, quantitative versions of training principles that can be incorporated into computer models) and training principles.

9. Theories of Tomography of Social Networks. This MURI began in FY10 and was awarded to a team led by Professor Patrick Wolfe of Harvard University. The goal of this MURI is to investigate theories for automatically analyzing heterogeneous, noisy, and incomplete multi-source data, and to infer information about individuals of interest and covert groups.

The MURI team will develop these theories using passive network observation and inference from traditional sources, as well as active sensing in a way that does not perturb the network as it evolves dynamically over time. In contrast to much prior work, this research places particular emphasis on the elicitation of metrics and models embedded in applicable sociological theory rather than simply on inference of latent structure in social networks. The effort has three focus areas, the first of which is metrics linking social structure to observable behavior. Two basic questions under consideration are (i) how is latent network structure manifested in observable data and (ii) how is observable data predictive of network structure. The second focus area is the interplay between individuals and groups as drivers of network dynamics. The third focus area is actionable intelligence from network models. In this area, the primary question is that of determining when is it possible to actively encourage (or disrupt) the formation of social structure. This effort responds to the Army need for time-sensitive and dynamic targeting of networks of hostile adversaries.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY10.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Modern Random Number Generation for High-Performance Computing. A Phase I STTR contract was awarded to Frontier Technology and to Silicon Informatics to investigate numerical methods for scalable random number generators and to develop algorithms and computer software that can be implemented for military and commercial simulation applications.

Monte Carlo simulation has proven to be an indispensible technique for developing robust models over both low- and high-dimensional parameter spaces, helping simulation become widely recognized as the third major component of scientific discovery and development, co-equal with experimentation and theory. With the advent of scalable parallel processing architectures, the need has become apparent for random number generators (RNGs) that are both parallel (capable of executing on multiple processor threads simultaneously without coherence) and scalable (capable of running on a variable number of processors, currently into the thousands and in the near future into an order of magnitude more, without coherence). Most modelers are aware of the danger of coherence in RNGs: stochastic models generate results with high degrees of periodic correlation between sections of output, reducing multiple runs to just replications of a small number of runs. In the worst case, this can effectively reduce the number of trials to just one, and is even more dangerous since the coherence is often masked in the high dimensionality of the problem and is not easily noticed. While some work has been done in parallel RNGs, all of the results to date are particular to a given architecture and size and are not universally scalable or distributed. This project seeks to develop a scalable implementation encoded in a standard software routine or set of routines that can be distributed within standard high performance computing (HPC) libraries for Monte Carlo computations and stochastic simulation on parallel, distributed, and Grid-based computing platforms. This will enable Army modelers access to algorithms and libraries on modern architectures that provide reliably independent, uncorrelated runs for simulations which rely on stochastic simulation.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goal of the HBCU/MI and TCU programs is to enhance the research capabilities and infrastructure at minority institutions, and to increase the number of under-represented minority graduates in the mathematical sciences. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Fractional Differential and Integral Inequalities with Applications. This HBCU project began in FY10 and is led by Professor Donna Stutson at Xavier University of Louisiana. The overall scientific goal of this study is to develop the theory of fractional differential and integral inequalities. Many physical applications are commonly modeled by fractional differential equations (FDEs) and stochastic fractional differential equations. Some fractional differential operators, like the Riemann-Liouville operator, are more challenging than others (such as the Caputo operator) since the former occurs in forms that can introduce singularities in the FDE. Within the past two years, certain basic results of FDEs and related inequalities have been developed, yet, certain fundamental analogues such as the variation of parameter method remain unsatisfactory. This project plans to extend the theory of differential and integral inequalities to fractional boundary value problems and fractional reaction diffusion equations with initial and boundary conditions. The core idea is to establish new fractional differential and integral inequalities which can be used to better understand the qualitative and quantitative properties of a variety of FDEs.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Mathematical Sciences Division managed five new DURIP projects, totaling $1.1 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including efforts to model sharp-

interface flows, to solve coefficient inverse problems, to enhance situational awareness in urban environments, and to achieve spatio-temporal event pattern recognition.

I. DARPA Geometric Representation Integrated Dataspace (GRID)

The vision of the GRID program is to establish the theoretical foundations and pragmatic implications of a compressive representation format for high-resolution 3D data of all sensor modalities. The envisioned GRID format would accurately encode the 3D geometry and surface properties of objects at various spatial scales and would provide efficient storage, application, and exchange throughout multiple industries. There have been numerous attempts, often independent and industry-specific, to efficiently capture 3D geometry and surface properties. This program seeks to unify disparate approaches in all three stages, namely, data format, encoding and rendering in automatic procedures. While there is strong interest in 3D land topography, this program also considers other areas such as manufacturing and biomedicine. The Mathematical Sciences Division has identified and initiated three pilot projects using DARPA funds to support the GRID program. In addition, many of this program's goals are complementary to the research directions pursued by Division's Theories of Dynamic Modeling of 3D Urban Terrain MURI.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Mathematical Sciences Division.

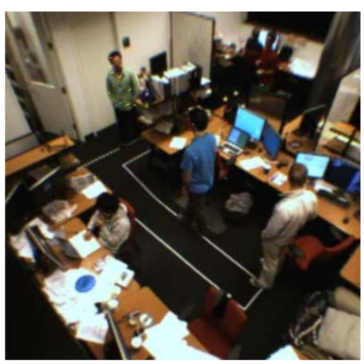
A. Distributed Information Fusion of Object Locations, Paths and Identities

Professor Leonidas Guibas, Stanford University, Single Investigator Award

The goal of this research is to investigate computational mechanisms for accurately tracking and estimating properties mobile objects (*e.g.*, people, vehicles) in cluttered environments under conditions with imperfect information, including occlusion (see FIGURE 1A). The information may concern simple attributes of individual agents in isolation, such as their color or size, or they may record events where multiple agents interact. Information is always obtained at discrete events that correspond to encounters between sensors, mobile agents, and their environment. The research uses 3D tracks of salient feature points obtained from distributed camera stereo pairs. It associates object tracks and identities via distributions over a symmetric group, avoiding the standard *n*! combinatorial complexity of truncated (low-frequency) Fourier transforms (see FIGURE 1B). Parametric and non-parametric filters for joint location and data association are used and, for scalability, distributions are factored into smaller independent components in Fourier domain.

The investigator has developed procedures that yield linkages of physical objects based on tracks (evidence of underlying physical and social networks) that other procedures are not able to identify, specifically linkage of geometrically distant objects (home and office of a person and linkage of these with other places). The procedures are motivated by physical sensing, but apply equally well to encounters in virtual or mixed cyber-physical environments. This research responds to the Army need for recognition, tracking and monitoring of civilian-like targets in difficult urban settings with occlusion and clutter. These techniques are most applicable to settings where there is high mobility in constrained environments leading to repeated observations of the same entities (agents, or parts of the environment). Examples of these scenarios that most commonly meet these characteristics include the deployment of simple sensors an urban environment to monitor activities, and sensors being carried by friendly forces to map a region.

A



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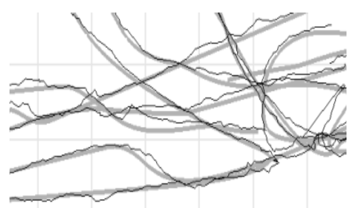

FIGURE 1

Designing computational mechanisms for tracking mobile objects in cluttered environments. (**A**) A cluttered office environment is shown in which tracking takes place and in which relations between objects based on tracks (evidence of social networks) can be established. (**B**) The plot displays identity-managed tracks by which the relations between objects are established; tracks are in the horizontal xy-plane (latitude-longitude plane) in the office environment of (A), seen from vertical.

B. Learning Geometry and Representations without Explicit Segmentation

Professor Guillermo Sapiro, University of Minnesota, Single Investigator Award

The objective of this project is to develop a comprehensive framework for 3D object recognition and identification from partial information due to occlusions or incomplete acquisition. In FY10, as components of

this framework, the investigator developed dictionary-learning techniques for image and shape enhancement and analysis, shape segmentation and analysis in video, 3D articulated object recognition and classification, channel network extraction, and 3D brain image analysis. The framework depends on the ability to match a 2D image with a 3D image (see FIGURE 2). The approach starts from sparse representations (*i.e.*, representations that do not have a lot of independent components). A library of 3D objects of interest is the priors for the method. The distributions of distances of voxels (*i.e.*, computational cubes in space) can be used for 3D pose recognition (see FIGURE 3). The investigators have also successfully (i) developed techniques for dictionary learning, including on-line learning (code made public and transferred to DoD organizations), (ii) designed a complete pipeline for object segmentation in video that was incorporated into Adobe's After Effects April 2010 release, and (iii) prepared an automatic framework for channel extraction from LIDAR (Light Detection And Ranging), incorporated into geoscience data analysis software packages. Recognition and identification for 3D articulated object recognition are accomplished by maximizing the likelihood consisting of object fidelity (match 3D shape prior) and image fidelity (projection matches actual image). Extension to the detection of non-rigid symmetries in 3D objects was also achieved. The framework is robust to topological changes (*i.e.*, introduction or deletion of holes). This research enhances Army capabilities in target recognition and identification in cluttered urban environments.

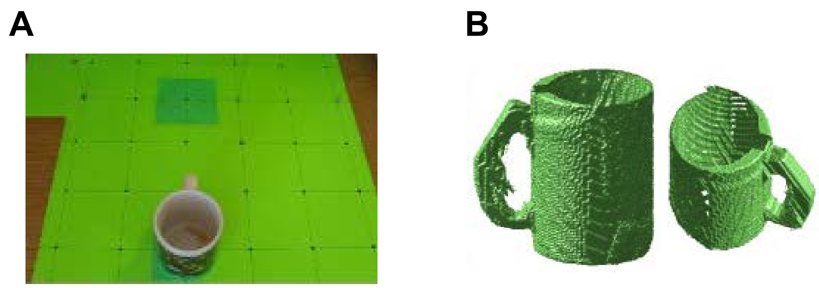

FIGURE 2

Potential application of learning geometry representations. One long-term objective of the project is to understand and develop frameworks for analyzing (**A**) a single 2D image and converting the results to (**B**) a 3D representation.

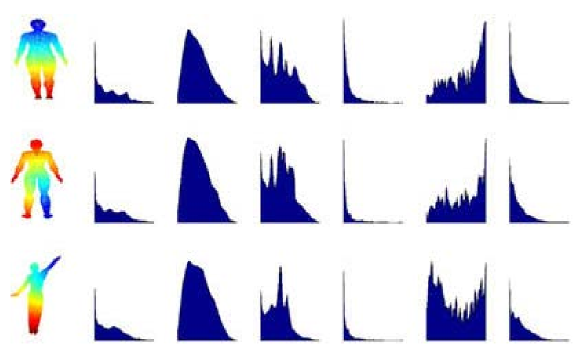

FIGURE 3

Image representation of 3D human poses. A greater understanding of learning geometry in complex environments could enable more accurate recognition of targets in cluttered sensor environments.

C. Mathematical Models to Compare Insurgent Activities to Urban Street Crime

Professor Andrea Bertozzi, University of California, Los Angeles, Single Investigator Award

The goal of this project is to develop principles for measuring whether two social groups are similar. The research involves both analysis of field data and constructing mathematical models, with a goal of developing a mathematical framework to connect observational data with basic mechanistic models. An important part of the research is the investigation of geospatial patterns (such as urban and rural terrain, location of routine activities of potential persons of interest and transportation routes) and clustering of events in space and time. Another

part of the research involves construction of dynamic models to begin to understand how to control and dissipate insurgent activity.

The investigators have demonstrated that improvised explosive device (IED) activity in Iraq is well represented by a self-exciting point process model, consistent with the dramatic temporal clustering of events in the Iraq Body Count (IBC) database. The key application of these models is to determine whether the characteristics of civilian urban street crime are close enough to those of insurgent activities (see FIGURE 4) that the former can be used in research to represent the latter. A better understanding of these processes will contribute to policy and security strategies to address the national security challenges posed by terrorism and insurgencies.

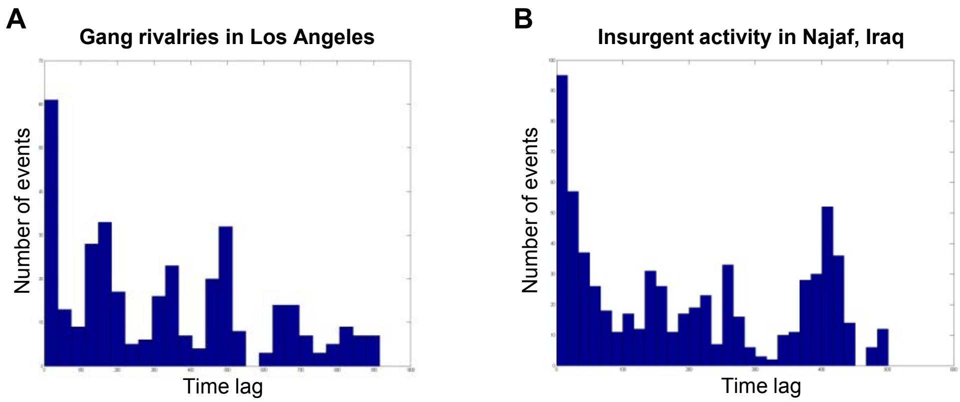

FIGURE 4

Comparing urban street crime with insurgent activity. Histograms of the number of events (y axis), such as IED activity or gang shootings are plotted vs. time between events (x axis) for (**A**) gang rivalries in Los Angeles and (**B**) insurgent activity in Najaf, Iraq.

D. Diffusion-Limit Theory and Network Dynamics
Professor Amarjit Budhiraja, University of North Carolina, Chapel Hill, Single Investigator Award

The objective of this project is to study stability properties and develop techniques for obtaining near-optimal control policies for a general class of processing networks. A typical processing system that is a network of buffers, service stations, and processing activities commonly arises from manufacturing, communication and computer networks (see FIGURE 5).

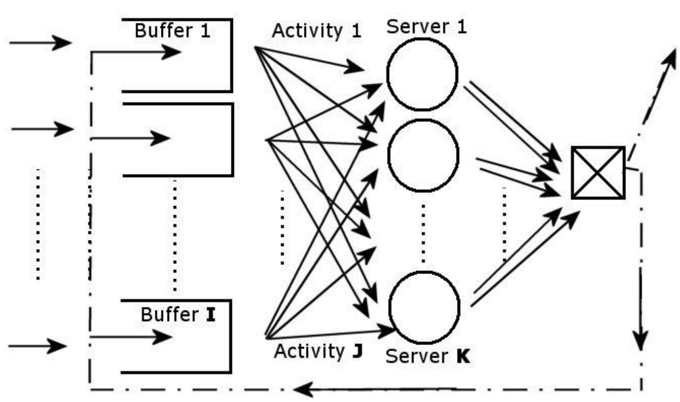

FIGURE 5

Schematic of a typical information processing network. A network with I buffers, J activities and K servers, in which jobs arrive in buffers and are served one at a time by a given server. An activity links a buffer with a server (*e.g.*, activity 1 corresponds to buffer 1, served by server 1). Networks such as this can be quite complex and may benefit from reduced operating models that may result from diffusion limit theory.

These processing networks can be quite large in terms of number of stations, buffers, and activities. Furthermore, the network topologies can be quite complex. Adding to the challenge, system managers can exercise dynamic control in the form of alternate routing, sequencing of jobs, and input control. The goal of a

system manager is to minimize some suitable cost function that could be given in terms such as inventory holding cost, throughput times, or server idle times. Although the networks of interest are too complex to be analyzed directly, one can obtain reduced models by using diffusion limit theory (DLT). The appeal of this approach is that in the limit, a lot of extraneous details are washed out and one is able to look at network dynamics in their "sharpest relief" as a (controlled) diffusion process. Control and stability issues for diffusion are significantly more tractable. Once these issues are resolved, one can go back and infer stability properties and good control policies for the underlying network.

Recent accomplishments include the calculation of stability conditions obtained using Lyapunov function methods and by deriving uniform moment bounds from the steady-state behavior of a broad family of generalized Jackson networks with non-Markovian statistics. There are well established numerical schemes for computing stationary distributions of reflected diffusion which, in view of this result, can be used to compute approximate steady state characteristics of the underlying networks of interest. In particular, the problem of optimal rate control for generalized Jackson networks has been studied. The PI has used a control problem for diffusion processes that was arrived at through formal heavy traffic considerations to derive provably asymptotically optimal rate control policies for the underlying physical networks. Using these results one can numerically construct policies that perform well over long periods of time by approximating the Hamilton-Jacobi-Bellman equation for the associated diffusion control problem.

In addition, the PI has obtained heavy traffic limit theorems for multiscale queuing networks of the approximating Markov chain. Systems with temporal variations of two types have been investigated. The first occurs at a rate much faster than typical interarrival and processing times while the second is much slower and manifests itself only over long periods, in relation to diffusion approximation time scales. Limit theorems established in this work allow the approximation of such large complex networks by reflected diffusions whose coefficients are modulated by the slowly moving background process and that also depend on the steady state distribution of the fast oscillating Markov chain. One application of these results is to the development of simple simulation approaches for large networks with a multiplicity of time scales.

E. Density Estimation and Anomaly Detection in Large Social Networks

Professor Rebecca Willett, Duke University, Single Investigator Award

When monitoring interactions within a social network, meetings or contacts between different members of the network are often recorded. The objective of the research effort, which led to a noteworthy FY10 accomplishment, is to use recorded meetings and contacts within a social network to determine (i) whether each meeting is anomalous, (ii) the likelihood of a given meeting occurring, and (iii) which other people are likely to interact with a given list of people. Many social network analysis approaches involve constructing a graphic representation of the network, where each vertex corresponds to a person and each edge corresponds to whether *two* people have met or interacted. This approach can be limiting because information about higher-order interactions (*i.e.*, group meetings with >2 people) is lost and representing a large group meeting as a series of pairwise interactions is a computationally-intensive process.

This project's research approach is a novel departure from the approach used by typical researchers in this field, by instead using *hypergraphs*. Hypergraphs continue the typical approach of using vertices corresponding to people, but with the addition of *hyperedges,* corresponding to the observed meetings, that connect any number of people in the network simultaneously (see FIGURE 6). Using this hypergraph framework, the investigators are not limited to simply analyzing the structure of a social network. Instead, the investigators can explore behavior patterns of the network members, form useful predictions of future social network activities, and identify activities that are outside the scope of "normal" network behavior. Within this framework, determining whether a meeting is anomalous or determining the likelihood of a given meeting corresponds to assigning a likelihood to each possible hyperedge. This approach presents significant opportunities for addressing challenges in social network analysis that are intractable using conventional tools. However, there is a computational barrier because in a social network with p people, there are 2^p possible meetings (*i.e.*, hyperedges), and enumerating all possible hyperedges would be prohibitive.

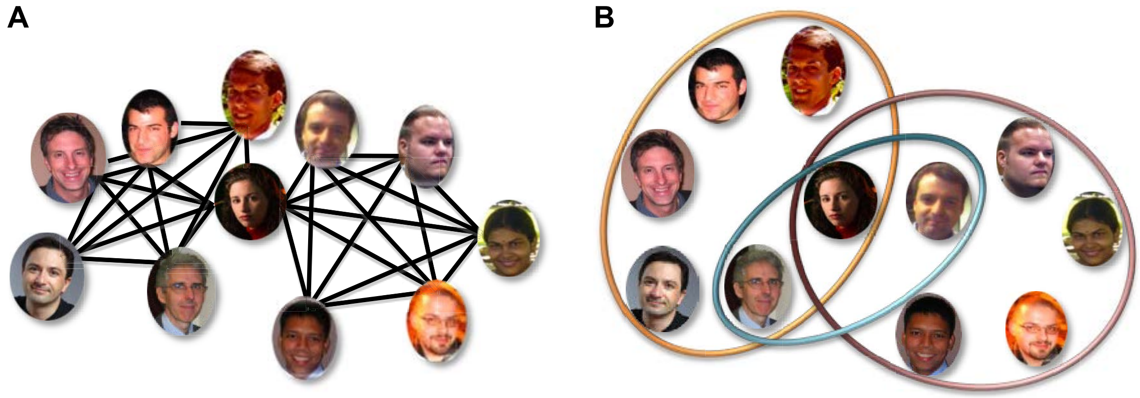

FIGURE 6

Traditional and hypergraph representations of a social network. In both (A) a traditional representation and a (B) hypergraph, people are represented as vertices; however, a hypergraph includes hyperedges that connect any number of people in the network simultaneously.

While the above hurdle is significant, there is nevertheless an opportunity to accomplish the predictive goals through benign yet simplifying assumptions. In one portion of the work, it is assumed that the probability distribution over possible meetings or hyperedges admits a *sparse representation* (*i.e.*, that the 2^p-dimensional distribution could accurately be approximated as the weighted sum of a small number of simple distributions). In this case, the sparsity could be exploited to ensure that the full probability distribution could be learned in at most $O(p^2)$ time, and as little as $O(p)$ time. This is a significant computational savings over other approaches, which would require $O(2^p)$ time. The results of this approach have proven to be optimal for a broad class of possible probability distributions over hyperedges or meetings.

In the second part of this research, the PI developed a *sequential* method for social network meeting prediction. The principle of this concept is that after observing t-1 meetings, one would like to generate a predictive probability distribution that reflects how likely one believes each potential future meeting to be. To address the computational hurdle describe above, one can restrict this predictive distribution to be a member of an exponential family of distributions, a broad class of distributions that has been used effectively in a wide variety of density estimation settings. After making a prediction for time t, the research team observed the next meeting and used it to assess the accuracy of the investigator's prediction. This procedure is repeated, and the goal is to ensure that the sequence of predictions is as accurate as possible. This approach is significant because (i) one can update the predictive density at each time t without having to retain all previous observations, resulting in very computationally efficient update algorithms, and (ii) one can prove that the sequence of predictive densities is nearly as accurate as the best possible sequence of predictions that could be made given full knowledge of both past *and future* meeting observations. Simulation results have shown that the performance of this method is substantially better than the best static threshold that can be chosen in retrospect with full knowledge of all observations (see FIGURE 7).

An important extension of this sequential approach is a novel method for detecting anomalous or unusual meetings. In particular, the investigator flagged meetings that have a very low likelihood under the learned predictive model. One of the chief challenges, however, is determining the threshold at which a likelihood is considered "low"; this threshold should result in meaningful detected anomalies for the end user. This approach is novel and significant because it allows the end user to provide feedback to the sequential algorithm regarding the accuracy of the declared anomalies, and then to use this feedback to adjust the threshold to a more appropriate level. In addition, the proposed approach is effective even when feedback is only offered for a fraction of the observations, reflecting the constrained resources of the feedback provider.

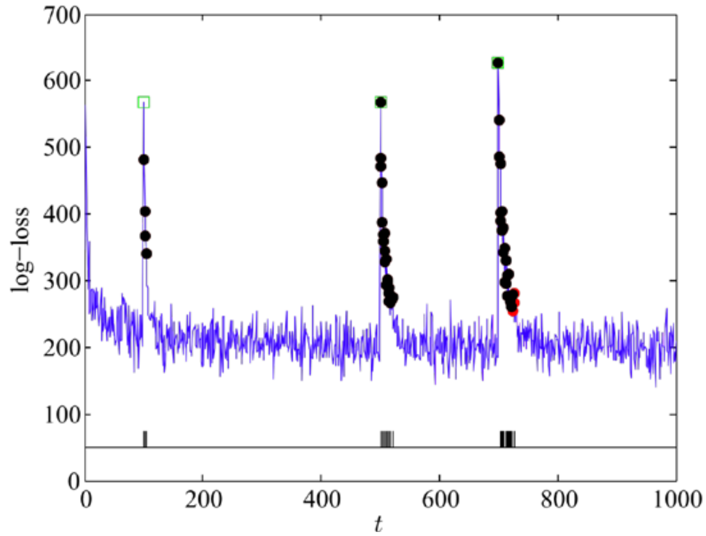

FIGURE 7

Sequential method performance versus static threshold. Simulations show that the performance of the sequential method is substantially better than the best static threshold that can be chosen in retrospect with full knowledge of all observations. The blue plot measures the inaccuracy of the prediction across time. At three different times (t = 100, 500, and 700), the behavior of the social changes and the predictions are highly inaccurate until the method adapts to the new "normal" network behavior. Black dots indicate truly anomalous meetings given past meetings; red dots indicate anomalous meetings that were undetected with the method. Black hash marks at the bottom of the plot indicate times at which the method received feedback from an end user. Even with this limited feedback, errors associated with this anomaly detection method are less significant than those detected with the best possible static, non-adaptive threshold.

F. Developing Multi-scale/Multi-physics Models Capable of Analyzing Advanced Energetic Processes

Professor Catalin Picu, Rensselaer Polytechnic Institute (RPI), Single Investigator Award

The objective of this project is to computationally integrate the nano- and mesoscales of detonation by modeling the physics on multiple scales that are relevant for hot spot formation. The theoretical approach begins by constructing atomistic models of RDX that include all covalent, Van der Waals, and electrostatic interactions. These are used to model entire crystals, which are then used to construct coarse-grained mesoscale representations. Computational complexity is kept tractable by reducing the number of degrees of freedom in the coarse model while preserving accuracy within specified bounds. The coarse-grained potentials are calibrated by an inversion procedure from the Boltzmann probability distribution function (PDF) and then used as the computational translation with the fully-discrete models. As computation proceeds, adaptive refinement and coarsening is used to maintain a specified measure of error (see FIGURE 8).

Professors Picu and Shephard at RPI have made several noteworthy research accomplishments in FY10. An *ab-initio* atomistic modeling effort was successful and modeling was accomplished by implemented a chemically specific potential for RDX in the LAMMPS molecular dynamics code from Sandia and testing it against numerical and experimental data, and by incorporating molecular rigid-body potentials in the atomistic models that were obtained from the ARL Weapons and Materials Research Directorate (ARL-WMRD). These two models, one representing all atoms in each molecule and the other representing molecules as rigid bodies, bracket the range of models intended for exploration. Crystal defect structure and mobility in RDX was modeled and implemented, and dislocation-phonon emission and coupling with the internal molecular modes was modeled. The PIs determined the conformers that are stabilized by these potentials and energy barriers for thermally-activated transformations between these conformers. In the mesoscale modeling effort, the interaction of voids and dislocations and void collapse under impact conditions was calculated, localized phonon modes (due to presence of defects or resonant modes) were modeled, and interactions between dislocations and the jerky dislocation motion were simulated. The potential long-term applications and benefits of this work to the Army include designer munitions that are effective, yet more stable for handling and storage purposes.

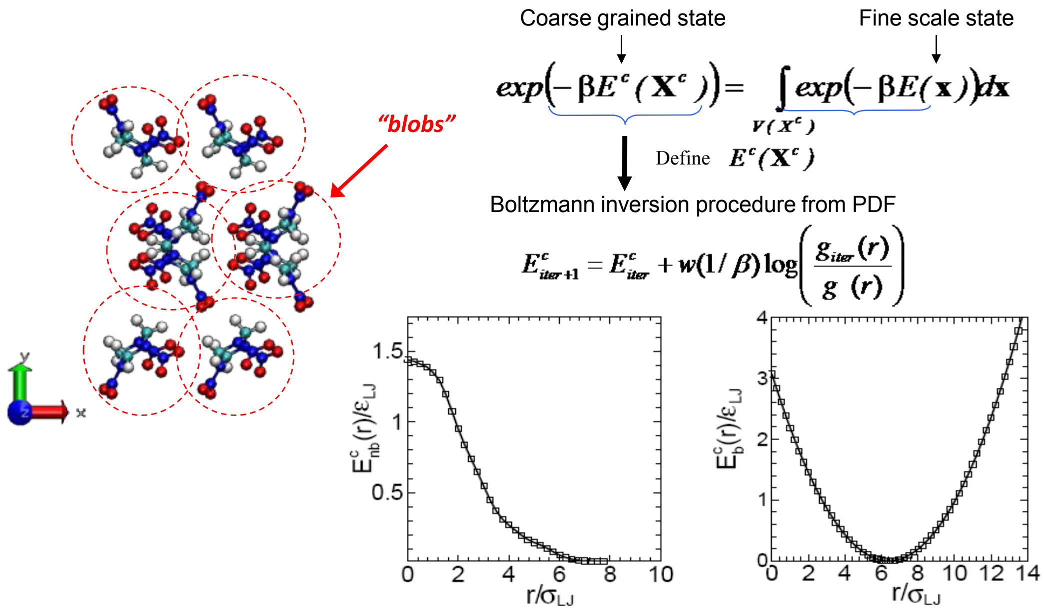

FIGURE 8

Schematic of procedure for creating a coarse-grained hierarchical model. The model is created by replacing entire molecules with "blobs," while interaction potentials, E^c, are defined between blobs. The potentials are calibrated based on the behavior of the atomistic model, a procedure called "Boltzmann inversion." The entire exponential term represents the total probability for the system (*i.e.*, a large molecule) to be in the state of energy E^c, that is equated to the sum of probabilities for the fine scale system to be in states defined by the energy E, which can be computed since the interatomic potential for the fine scale is known. These states of the fine scale system must be topologically compatible with the given/current state of the coarse model of the same molecule, which is the reason for integrating over V^c (a region of the coarse-grained phase space). The plots show coarse grained potential, non-bonded (nb) and bonded (b), for dense polymeric molecules.

G. Globally Convergent Numerical Methods for Coefficient Inverse Problems

Professor Michael Klibonov, University of North Carolina, Charlotte, Single Investigator Award

The goal of this project is to solve inverse coefficient problems that converge to the correct solution from almost any choice of initial iterant. Linear methods are almost universally used for these types of problems, as they rely on forming a linear cost function as the measure of error and then seek to minimize it. This approach inevitably possesses many local minima; therefore, unless the initial guess is close to the true solution (which is almost never the case), iterants will usually settle into these local minima, very often far from the true global minimum.

In FY10, the investigator has proven a convergence bound that holds for all initial iterants. It is of the form n^n and thus is similar in nature to bounds often found in regularization algorithms, and it is convergent for the first several iterations. However, it is ultimately divergent and therefore cannot be iterated arbitrarily and must be monitored. In practice, this makes the global algorithm useful for several iterations from an arbitrary initial iterant, and generates an approximation to the global minimum that can then be used in a faster linear method. This accomplishment provides a numerical inverse method that is both globally convergent and highly robust. The method works with limited data (*e.g.*, backscatter data), while comparison with linear methods shows that the latter typically does not work well with this type of incomplete data. The newly-developed theorem rigorously proves, and experiments numerically verify that no prior knowledge or initial guess is required.

The investigator has demonstrated high quantitative accuracy in imaging from blind experimental data in test cases provided by ARL-SEDD (see FIGURE 9).

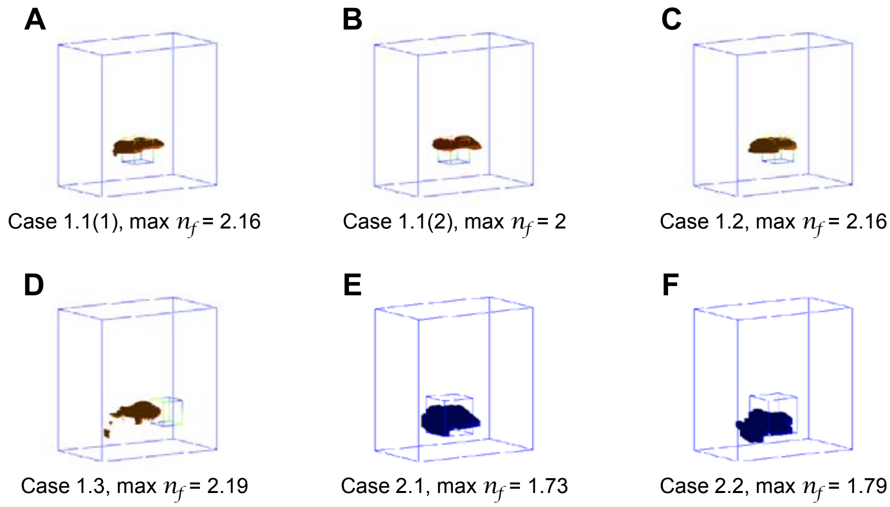

FIGURE 9

Reconstructed images of unknown targets. (A-F) Six blind-blind trials were calculated from data provided by ARL-SEDD, reconstructing images of unknown targets in unknown locations. Targets are cubes of a material of higher dielectric constant embedded in a material of lower dielectric constant. The small dashed cubes are the true target outline; solid images are the reconstruction at an intermediate stage before mesh refinement; mesh refinement and further iteration reconstructs the targets nearly exactly.

These test cases demonstrate that the method can compute not only step changes in permittivity (object boundaries), but also permittivity values (object constitution). The potential long-term applications and benefits of this work for the Army include the capability to not only locate the boundaries of objects from backscattered data, but to also determine the composition. For example, this could be useful in determining whether imaged objects, such as buried or occluded objects, are comprised of explosive ingredients.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Portable 3D Mapping of Building Interiors

Investigator: Avideh Zakhor, University of California, Berkeley, Single Investigator Award
Recipient: ARL Vehicle Technology Directorate (ARL-VTD)

The objective of this effort is to develop the algorithms and architecture for photo-realistic rendering of 3D interiors of buildings and navigation in areas where Global Positioning System (GPS) navigation is unavailable. The algorithms and architecture are designed for off-the-shelf sensors (*e.g.*, laser scanners, video cameras, inertial measurement units). Data is continuously acquired as an operator walks or a robot moves, rather than in stop-and-go fashion by parking equipment at discrete locations. The indoor localization algorithms do not presume GPS accessibility and do not use wheel odometry. These algorithms and architectures were implemented in an ARL-VTD system for a wheeled mobile robot, in which 3D point clouds are generated and planes (walls, etc.) are automatically detected; camera imagery is captured for external use. This system allows the robot to autonomously navigate. Software items delivered with the hardware system were a framework for on-line and off-line localization and algorithms for pose recovery, recognition of planes and features, loop closure, backward correction in time, merger, fusion and registration of multiple sub-models. Analysis deliverables include characterization of scalability, error analysis, convergence properties and optimality analysis. Tests of this system in typical environments confirm its accuracy (see FIGURE 10), and this technology has transitioned to ARL-VTD for further testing in robotic navigation and mapping in GPS-denied environments.

A **B**

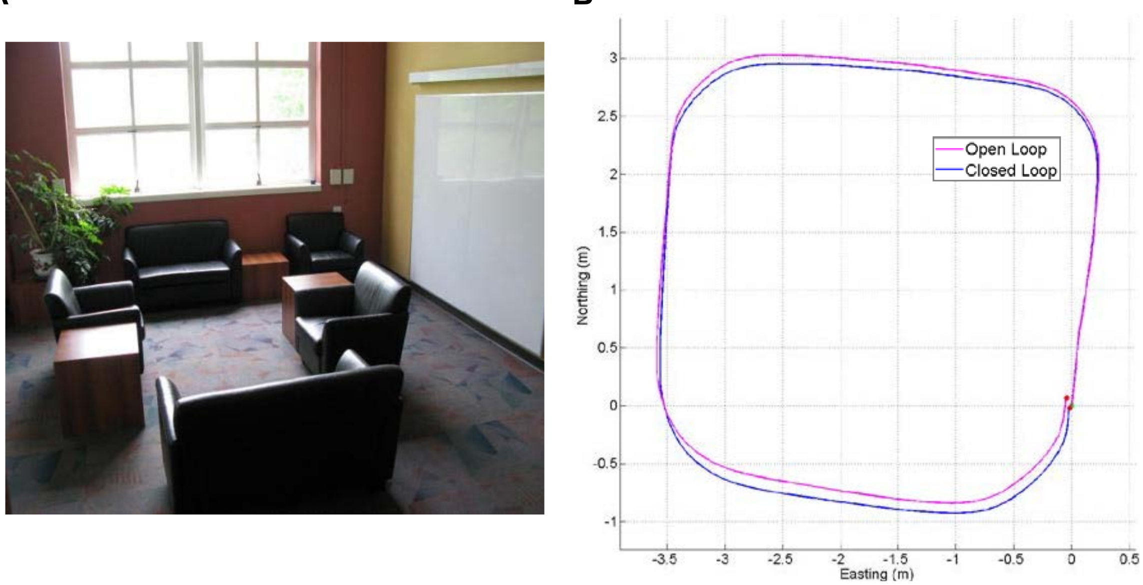

FIGURE 10

Testing algorithms for photo-realistic 3D rendering and navigation. (**A**) A cluttered office environment was chosen because of its medium complexity, and is the location where autonomous navigation was tested. (**B**) Robot path in the horizontal xy-plane (latitude-longitude plane) in the office environment of (A) seen from vertical. The closed-loop path is in blue, and the open-loop path is in red. The path shows avoidance of the obstacles (furniture) in the room. Note that the open-loop path is almost as good as the closed-loop path.

B. Spatial-Temporal Event Pattern Recognition
Investigator: Aram Galstyan, University of Southern California, MURI Award
Recipient: National Counter-Terrorism Center

Under this MURI project, Professor Galstyan has been investigating new mathematical theory and techniques for identifying and tracking covert activities of hostile agents. The overarching goal is to develop scalable and accurate methods for adversarial activity detection based on high-clutter data. Part of the research has focused on detecting activities in a virtual Hats World, which is a proxy for various intelligence analysis problems. The goal is to identify and neutralize the malicious agents before they can do harm, based on noisy observations about agents and their activities. In addition to algorithmic development, the project is testing analytical methodology that will allow understanding the properties and limitations of inference algorithms. The researcher has already successfully: (i) developed a Coupled Factorial HMM based for tracking the agents and approximation schemes for feasible tracking, (ii) validated the framework for large (more than 1000) agents, (iii) developed a Partially Observable Markov Decision Process (POMDP) framework for designing efficient security policies that are grounded in a Decision Theoretic approach, (iv) developed theoretical models to quantify one's ability and limitation to infer certain stochastic processes, and (v) developed a theoretical model to understand the limitations of group detection algorithms on graphs.

The research contributes to the overall Army objectives by developing methods for detecting certain dynamical processes that unfold on networks, which go beyond the static pattern detection paradigm. Although there is a large body of work on plan and activity recognition, most approaches are limited in scale and scope. The present approach addresses the shortcomings of previous work and will be used to develop scalable activity detection algorithms that will be suitable for larger and more realistic systems. Furthermore, this theoretical analysis allows understanding whether there are fundamental limits on one's ability to infer certain stochastic processes, and how to quantify those limits. In addition, this research will produce a set of scalable algorithms and practical tools that can be used by the intelligence analysis community. Furthermore, this theoretical work might lead to a different type of inference paradigm, Active Learning. The final product of the proposed research will include a set of algorithms for detecting hostile activities in high-clutter transaction data, and an underlying theory of detection of dynamical processes in such data.

Based on this MURI work, this research will transition to the National Counter-Terrorism Center, through which the researcher won an award "*Hybrid Probabilistic/Incremental Search Approach for Detection and Tracking of Adversarial Activities.*" The main objective of this project is to develop prototype models and a corresponding software toolkit to aid intelligence analysis. A particular emphasis will be put on ability of the models to predict adversarial behavior observed in real data.

C. Computer-Aided Design of Drugs on Emerging Hybrid High Performance Computers
Investigator: Michela Taufer, University of Delaware, Single Investigator Award
Recipient: ARL-CISD

Molecular dynamics (MD) simulations are important in chemical research as they can provide an atomistic view of chemical systems and processes not available from experiments, while the Coarse-Grained Monte Carlo (CGMC) method is a multi-scale stochastic mathematical and simulation framework for spatially distributed systems important for studying catalysis, surface diffusion, and cell membrane receptor dynamics. The goal of this project is to validate computational methods and to design and implement computational tools incorporating Graphics Processing Units (GPUs), to be used for biomedical problems such as drug design.

Using GPUs, this project has provided a MD computer code having increased computational power enabling explicit simulation of solvents, as well as a parallel CGMC code for studying scalability and scheduling issues related to domain decomposition of molecular simulations using multiple GPUs. In addition, large-scale numerical simulations performed on parallel systems tend to be very sensitive to cumulative rounding errors and can result in different answers depending on platform and number of parallel units used. Thus, this project also provided new composite precision floating point arithmetic libraries and associated algorithms for GPUs that combine double precision accuracy with single precision performance by defining addition, multiplication, and division in terms of multiple single precision additions, subtractions, and multiplications as well as a single precision floating point reciprocal, at the same time keeping track of inherent error as the simulation evolves.

A combination of parallelism and composite precision arithmetic on GPUs shows great promise in improving performance and reliability for large-scale simulations in general (see FIGURE 11) and for drug design in particular. These methods can significantly reduce the time required to find cures and vaccines for viruses and bacteria used as bio-weapons, lower the cost of new vaccines, and increase the effectiveness of existing cures. Researchers at CISD are in the process of evaluating the algorithms resulting from this project for use in solving reproducibility and stability issues, as well as domain decomposition of simulations across multiple GPUs for a variety of applications and are looking into computational drug design of small molecular therapeutics against bacteria and viruses. However, the methodologies resulting from this project are transferable across applications and thus provide Army scientists in general with important insights on how to migrate large-scale simulations on GPU clusters.

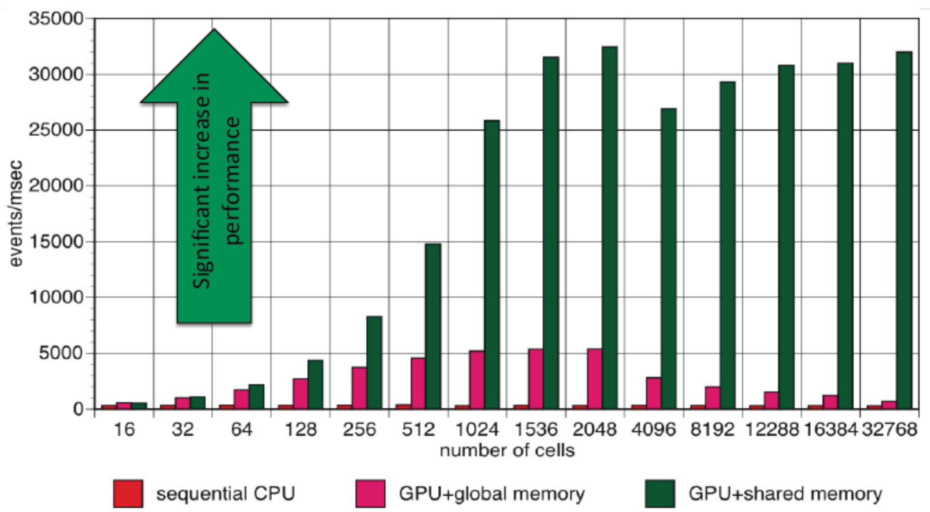

FIGURE 11

Computational tools incorporating GPUs superior to sequential CPU analysis. Performance results for parallelization of Tau-Leap Coarse-Grained Monte Carlo simulations on GPUs compared with simulations on sequential CPUs.

D. Reduced Order Modeling for Hydrodynamic Code

Investigator: Carl Kelley, North Carolina State University, Single Investigator Award
Recipient: Engineer Research and Development Center (ERDC), Vicksburg

The objective of this project is to generate a reduced model for inverse problems in saturated flow using principal orthogonal decomposition (POD). This research could ultimately allow the estimation of parameters that govern groundwater flow. The parameters of most concern are hydraulic conductivity and the measure of velocity of a liquid through a porous medium. The computational cost of an adaptive hydrology code (ADH) field-scale simulation in three dimensions is high, and it is important to reduce the number of expensive calls to the simulator. This is one of the reasons why the group at ERDC is not using methods like genetic algorithms or simulated annealing for calibration. Methods based on nonlinear least squares, however, miss the global features of the problem, and may converge to local minima that result in poor calibrations. This project provides a low cost approach to remedy this limitation, by providing a surrogate model or response surface to approximate the expensive objective function, minimize the surrogate with a global optimization method, and then sample the expensive function near one or more local minima of the surrogate.

The investigator is using a POD surrogate model, using a basis built from several runs of the simulator, extracting a useful low-dimensional subspace with an eigenvalue calculation. The algorithm uses a basis taken from the sensitivity vectors that can be efficiently computed within finite element simulators such as ADH. This technology transfer involves the integration of a well model into the POD formulation, and then integration of both into ERDC's production ADH code. The well model is required because the problems of interest at ERDC have integrated flux boundary conditions and the well model maps those boundary conditions into pressure boundary conditions (see FIGURE 12).

The aim is to solve the following equation:

$$\nabla \cdot (K \nabla h) = f \text{ in } \Gamma$$

But with the boundary condition:

$$\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_Q$$

Where:

$$\begin{aligned} \Gamma_D &= \Gamma_{d_1} \cup \ldots \cup \Gamma_{d_{Nd}}, \\ \Gamma_N &= \Gamma_{n_1} \cup \ldots \cup \Gamma_{n_{Nn}}, \\ \Gamma_Q &= \Gamma_{q_1} \cup \ldots \cup \Gamma_{q_{Nq}}, \end{aligned}$$

And:

$$\begin{aligned} \Gamma_{d_i} &\Rightarrow \quad h = \alpha_{d_i} \text{ on } \Gamma_{d_i}, \\ \Gamma_{n_i} &\Rightarrow \quad \frac{\partial h}{\partial n} = \beta_{n_i} \text{ on } \Gamma_{n_i}, \\ \Gamma_{q_i} &\Rightarrow \quad \int_{\Gamma_{q_i}} \frac{\partial h}{\partial n} \, dS = \phi_{q_i} \text{ on } \Gamma_{q_i} \end{aligned}$$

FIGURE 12

Total flux boundary condition implemented in ADH code via reduced-order POD methods. The first equation governs groundwater flow through nonhomogeneous media, and the following equations, particularly the last three, illustrate the mapping of flux boundary conditions into constraints on the pressure field.

The development and implementation of the total flux boundary condition is of interest not only in optimization research, but also in the full ADH code. This boundary condition also serves as a useful well model for other applications. ERDC-Vicksburg has integrated this algorithm into its production ADH production groundwater modeling code and will use it as an inexpensive source of function calls in order to solve the sequence of minimization problems involved in parameter estimation calculations. This improves solution speed by about a factor of ten, which now makes possible the use of genetic algorithms for this kind of parameter estimation. The projected long-term benefit to the Army is enhanced capabilities for well modeling that will result in fast, high-fidelity predictions and groundwater remediation planning for the Army Corps of Engineers.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Algorithmic and Software Infrastructure for Extension of Indoor Portable 3D Mapping System

Professor Avideh Zakhor, University of California, Berkeley

The goal of this research is to design algorithmic and software infrastructure for the development of navigation algorithms that were previously designed from 2D with three-degrees-of-freedom localization, to 3D with six-degrees-of-freedom localization. These algorithms will enable the estimation of the full pose for the sensor platform (*x*, *y*, *z*, roll, pitch, yaw), thereby enabling the rover to operate in non-flat terrain, such as caves, or any situation in which pitch and roll are not negligible. The current modeling algorithms and software will also be extended to capture imagery from the on-board cameras and to texture-map the model with those images.

It is anticipated that in FY11, this research will lead to the demonstration of (i) 3D localization by a "2xICP+IMU" algorithm based on two applications of an iterated closest point (ICP) scan matching algorithm for *x*, *y* and yaw ("2xICP") and on an inertial measurement unit (IMU) for *z*, pitch and roll, (ii) the design and implementation of the image capture pipeline, and (iii) the texture mapping of the detected planes. Algorithms and software using three degrees of freedom, for navigation and localization in complex environments such as staircases, have already demonstrated the feasibility of this approach (see FIGURE 13). Testing of the extended algorithms and software will take place in fully 3D environments with nonhorizontal floors and no assumption of planarity of the floors.

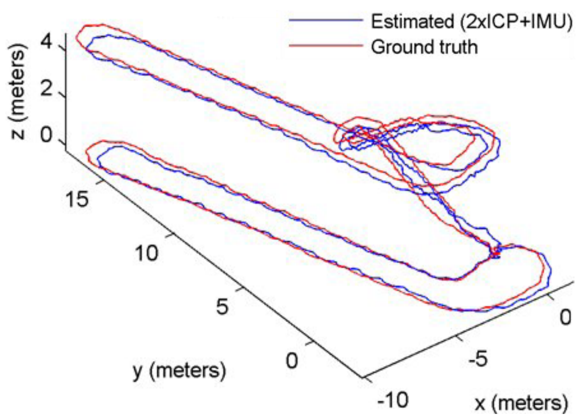

FIGURE 13

Localization and navigation in a simulated complex environment using algorithms with three degrees of freedom. The path of a robot was assessed in an office building with a staircase (chosen because of its medium complexity) in which autonomous navigation takes place. The path estimated by the theory produced by this project (blue) is an excellent approximation of the ground-truth path (red). The anticipated accomplishment is the extension of this to more complex environments.

B. Extensions of Signature Theory

Professor Frank Samaniego, University of California, Davis

This project is investigating the joint behavior of systems with shared components using the structural, stochastic, and statistical reliability theory for systems and networks. The results of this study may enable extensions of the concept of "system signature" to bivariate situations in which pairs of systems share some components and thus have dependent lifetimes. The problem explored here is motivated by examples of the sharing of components in the design of selected computer networks. In order to study the performance characteristics of pairs of systems with shared components, one needs to have analytical entrée into the joint distribution of their lifetimes. While some progress of such problems has been made in selected parametric

settings (*e.g.*, the Marshall-Olkin multivariate exponential model), the investigator's approach to the problem is fully general and removes parametric assumptions. The primary barrier to the envisioned work in this area is the absence of precedents in dimensions greater than one for representations of the type sought. The potential for generalizing signature representations to higher dimensions was quite difficult to predict. Even with such representations in hand, the possibility of identifying conditions under which a bivariate ordering exists between two pairs of systems, each with shared components, was seen as an uncertain exercise.

It is anticipated that in FY11, representations will be prepared for the joint distribution (and joint reliability function) of pairs of coherent systems with shared components under the assumption that all components have i.i.d. lifetimes. The expression derived for the joint distribution G, for example, depends on a pair of matrices S and S*, each of which has total mass (the sum of all its elements) equal to 1. The pair (S, S*) is referred to as the joint signature, and, under the assumption i.i.d. component lifetimes, it is shown to be independent of the underlying component distribution. In the problem of making stochastic comparisons between two pairs of such joint systems, the project provides, in two separate and quite different settings, sufficient conditions on the joint signatures to ensure that the two joint lifetimes satisfy a specific bivariate stochastic ordering. Similar results are obtained in studying the ordering of two joint reliability functions. Although the occurrence of systems with shared components is quite common (a simple example being two computers dependent on a common server), a general and flexible theory for assessing the joint stochastic behavior of these systems has not been available previously. The representations expected from this research will break new ground in this area, providing a tool for describing the performance of pairs of systems whose components have i.i.d. lifetimes with some components in common. The utility of these representations is demonstrated through the stochastic ordering results that follow and shed light on the relative behavior of two such joint systems.

The abundance of circumstances in which pairs of engineered systems have components in common suggests that a general theory for the joint stochastic behavior of such systems is needed. The application of joint signatures to comparisons between such systems will contribute toward this need in existing reliability analysis. The research results will have significant impact on the design of weapon systems for the Army and DoD.

C. Adaptive Networks Foundations: Modeling, Dynamics, and Applications

Professor Leah Shaw, William and Mary University

The objective of this project is to study node states and changes in static networks. Interconnected systems in a variety of areas are often modeled using a network approach. While the structure of static networks has been well-studied, when node states and links between nodes change over time, the feedback relationship between the node dynamics in the network and the changing pattern of interactions between nodes is often ignored. The long-term applications of this work may extend the tools of networks to adaptive social networks, focusing on the spread of infectious disease as the primary example, with individuals as nodes. The goals of the project include extending previous models to incorporate more realistic network structure, studying the extinction of diseases, developing control strategies for epidemics on adaptive networks, and developing tools to quantify adaptive network properties. The theoretical approach is based on a compartmental differential equation model for individuals in which compartments represent disease status, with each individual in either the susceptible (S), infected (I), or recovered (R) compartment, and individuals linked to create a social network (see FIGURE 14).

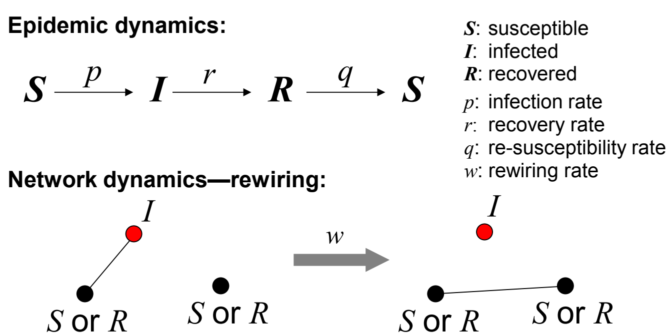

FIGURE 14

Epidemic and network dynamics model of disease spreading. The basic compartmental model (assuming reinfection is possible) is shown at the top, and the network dynamics model is illustrated at the bottom.

In an adaptive network, individuals change their social connections in response to the spread of an epidemic and these changes in network topology affect the subsequent spreading of the disease. Thus, as opposed to a standard epidemiological model, an individual avoids contact with an infected individual by disconnecting from the infected individual at a certain "rewire" rate and connecting to either a susceptible or recovered individual.

It is anticipated that in FY11 this research will lead to algorithms that capture increased realism in network structure and disease avoidance. Previous models for epidemics in adaptive networks have not accounted for the local community structures that occur in real social networks. As a first attempt to address the role of community structure, a model for an adaptive network containing two heterogeneous communities has been constructed, with the link rewiring rules adjusted so that the two communities are maintained throughout the evolution process. Characterization of this model, including epidemic persistence and bifurcation structure, will be achieved by systematic study of the dynamics of the two community system for a variety of network geometries and parameter values. In addition, current models assume that individuals are well-informed about their neighbors' disease status and their need to protect themselves from disease. This project considers the more realistic simultaneous spread of both the epidemic and information *about* the epidemic and will determine how these new effects alter the disease dynamics and prevalence.

Another anticipated accomplishment for this project is in the area of epidemic extinction. Having applied analytic and numerical techniques to find the most probable path to epidemic extinction and extinction rate to epidemics spreading in well-mixed systems, this project will extend the techniques to static and then adaptive networks. The effect of control strategies will be determined, including the previously studied pulsed vaccine control on epidemic lifetime (see FIGURE 15).

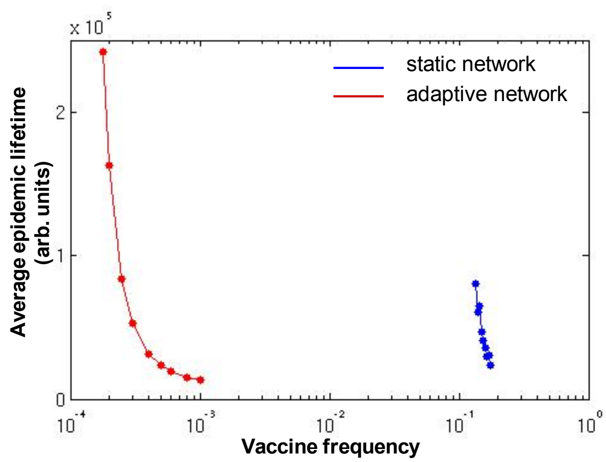

FIGURE 15

Dependence of endemic state average lifetime on vaccine frequency v under random pulsed vaccination of susceptibles. Two orders of magnitude less vaccine application is needed to drive the epidemic to extinction in the adaptive network case than in the static network case. Vaccine control is more effective in adaptive networks due to an interaction between the adaptive network rewiring and the vaccine application. This is an example of the wider class of control strategies that this project anticipates being able to predict.

As adaptive social networks are ubiquitous in both the Army and society, these anticipated accomplishments will have wide-ranging long-term applications and benefits. With respect to the social networks specifically considered in this project, likely results are improved policies on military troop movement in the presence of infectious disease as well as improvements in general public health policies. More generally, the mathematical tools developed for use with adaptive social networks may be applied to other types of adaptive networks such as communications systems and groups of unmanned autonomous vehicles.

D. Fast, Multiscale Algorithms for Wave Propagation in Heterogeneous Environments

Professor Thomas Hagstrom, Southern Methodist University

The goal of this project is the development of algorithms for the study and simulation of waves in the time domain. Wave propagation problems are fundamentally multiple scale problems, with relevant dimensions

ranging from the detailed structure of scatterers to the wavelengths to the propagation ranges. This fact poses a stiff challenge to computational technique as the uniform resolution of all scales present is unfeasible even for petascale computers. Thus this project seeks to develop hybrid multiscale algorithms encompassing accurate and efficient methods for: (i) near-field domain truncation, (ii) evaluation of long-range propagators, and (iii) robust, high-resolution volume discretization in complex geometry. The research approaches involve evaluating and improving methods in all three categories and pursuing integration and application to true multiscale simulations. Although the primary focus is on general purpose algorithms rather than specific applications, the central importance of wave physics in a wide variety of fields and the multiscale nature of waves themselves make them the tool of choice for communicating information and probing materials for foreign objects or defects.

It is anticipated that this research will establish a new type of computational boundary condition that overcomes current difficulties in achieving controllable accuracy at small cost, and of being able to put rigorous *a priori* bounds on the computational cost of achieving a pre-specified accuracy. The most basic multiscale problem in wave theory is the radiation of energy to the far field—effectively to infinity in mathematical models. Computationally, one requires a near field radiation condition, which provides controllable accuracy at small cost. This problem is of fundamental importance and there is a huge body of literature on it. No fully satisfactory solution currently exists, even for the simplest case of isotropic systems in homogeneous media. In particular, accurate and efficient methods based on compressions of the nonlocal radiation kernel are not always easy to implement and require restricted boundary shapes, while local methods such as approximate radiation boundary condition sequences and the perfectly matched layer (PML), suffer severe accuracy degradation over long time intervals (see FIGURE 16). This project anticipates achieving a solution to these barriers.

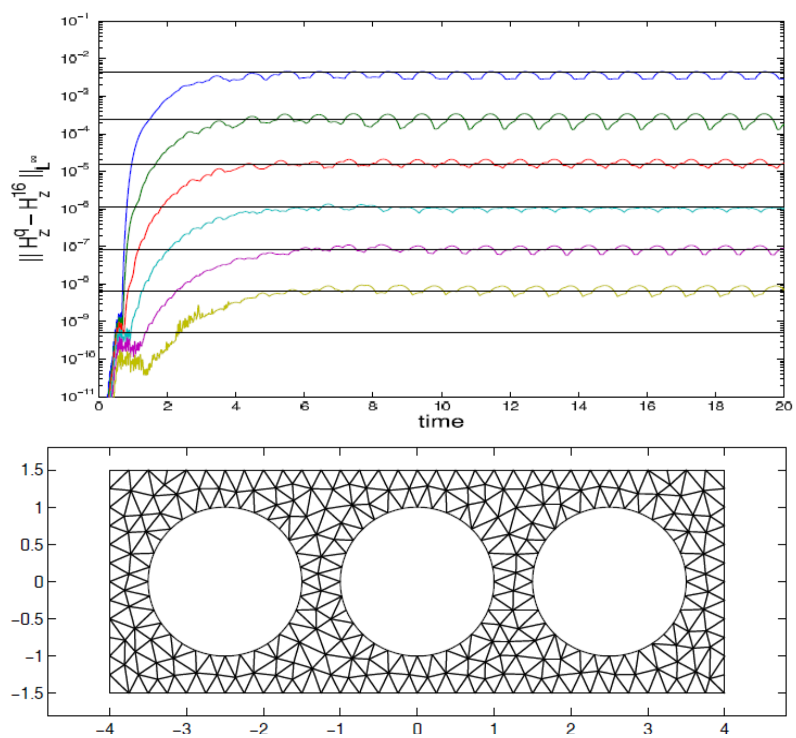

FIGURE 16

Preliminary results from scattering of a pulsed plane wave by three perfectly conducting cylinders. The boundary condition order is P = 4 : 2 : 14. Estimated and actual errors are compared; the method seems to promise controllable error that does not degrade over time. The spatial discretization of the Maxwell system is by a discontinuous Galerkin method with degree 10 polynomials.

Since waves possess a unified mathematical description and can be studied using common tools, these methods will ultimately have broad applications, both for the Army and for society as a whole. This will enable new Army capabilities for nondestructive testing of materials, faster and higher fidelity modeling of radar, signal, and other electrodynamic phenomena, and new capabilities for real-time, on-board analysis of field-based signals.

VI. DIVISION STAFF

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Program Manager, Probability and Statistics

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Program Manager, Biomathematics

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 10: MECHANICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Mechanical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research efforts to advance the Army and Nation's knowledge and understanding of the fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemical reacting flows, explosives and propellants, and actuation mechanisms and dynamics of complex systems of relevance to the Army and the DoD. More specifically, the goal of the Division is to promote basic research studies to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the design landscape used to optimizing systems, (iv) advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of complex systems as well as improving the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop fundamental understanding of the fluid dynamics underlying Army systems to enable accurate prediction methodologies and significant performance improvement, especially with regard to unsteady separation and stall and vortex dominated flows. Fundamental investigations in the mechanical sciences research program are focused in the areas of solid mechanics; actuation, dynamics and mechanisms; propulsion and energetics; and fluid dynamics. Special research areas have been continued in the Army-relevant areas of rotorcraft technology, projectile/missile aerodynamics, gun propulsion, diesel propulsion, energetic material hazards, mechanics of solids, impact and penetration, smart structures, and structural dynamics.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of properties and processes in mechanical sciences, the research efforts managed by the Mechanical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research in the mechanical sciences could provide understanding that leads to insensitive munitions, tailored yield munitions, enhanced soldier and system protection, novel robotic, propulsion, and energy harvesting systems, and novel flow control systems and enhanced rotorcraft lift systems. In addition, mechanical sciences research may ultimately improve Soldier mobility and effectiveness by allowing implementation of renewable fuel sources and new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary laboratory interactions of this Division are with the ARL Weapons and Materials Research Directorate (ARL-WMRD), ARL Vehicle Technology Directorate (ARL-VTD), ARL Sensors and Electron Devices Directorate (ARL-SEDD), the Joint IED Defeat Organization (JIEDDO), the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick Soldier RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division also facilitates the development of joint workshops and projects with Program Executive Office (PEO) Soldier and the Army Medical Research

and Materiel Command (MRMC). In addition, the Division often jointly manages research efforts with ARO programs in the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computer Sciences, and Life Sciences Divisions, through co-funded efforts, projects, workshops, and committees. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). Several international efforts are also coordinated through the International Science and Technology office in London (ITC-London) and the Pacific (ITC-Pacific).

B. Program Areas

To meet the long-term program goals described in the previous section, the Mechanical Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Solid Mechanics, (ii) Actuation, Dynamics, and Mechanisms, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program Area is to develop physically-based mechanics tools (theory, experiments, computations) for the quantitative prediction, control, and optimization of Army systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure. Solid mechanics research plays a crucial role in the prediction of strength, damage, and failure of Army materiel systems, structures and injuries of personnel under extreme loading conditions such as impact or blast as well as normal operating conditions. Research in computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing weight and volume, and its theories provide a strong link between the underlying physics of solids and the design of actual systems resulting in reduced development cost by minimizing the need for expensive system and field testing, and novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Multiscale Mechanics of Heterogeneous Solids, and (ii) Multiscale Mechanics of Biological Tissues. The goal of research efforts in the Multiscale Mechanics of Heterogeneous Solids Thrust is to extend the design envelope of current and future Army structures is predictive continuum damage and cohesive models with physical basis that are supported by *ab initio* and molecular dynamics modeling and experiments at the appropriate length and time scales. The objective of research in the Multiscale Mechanics of Biological Tissues Thrust is to understand how high rate loading of different durations and amplitudes may lead to cascading events starting at the cellular level that cause functional loss and impairment of human tissues and organs.

Research efforts in this Program Area are focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in our military systems. It is developing the methods needed to take advantage of recent advances in new materials technology, including nanotubes, nanocrystaline solids, and bio-inspired and hierarchical polymeric- and nano- composites. As a result of the long-term vision of the program, some future applications are yet unimagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor, unmanned aerial vehicles (UAVs), unmanned ground vehicles (UGVs), and munitions.

2. Actuation, Dynamics, and Mechanisms. The goal of this Program Area is to advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of materiel systems (*e.g.*, ground vehicles, rotorcraft, missiles, and projectiles) as well as to improve the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them.

This Program Area is divided into two research Thrusts: (i) Stability and Control of Interconnected Dynamic Systems, and (ii) Novel Actuation and Sensing Mechanisms. The Stability and Control of Interconnected Dynamic Systems Thrust is composed of five supporting and inter-related research topics: high degree-of-freedom dynamical systems, discrete and continuous systems, complex topologies, non-linear flexural dynamics,

and embedded state sensing. Advances in these areas are required to understand and improve the inherent capability of the organic structural components used in military systems and to enhance/enable subsequent applied research in energy harvesting, vibration and noise suppression, prognostics and diagnostics, and structural health monitoring. The Novel Actuation and Sensing Mechanisms Thrust consists of five research topics: distributed, multi-scale, multi-physics; multifunctional, reconfigurable, autoconfigurable, morphing, adaptive and/or stochastic mechanisms and actuation; high bandwidth/stroke mechanisms; direct chemical-to-mechanical conversion (*i.e.*, artificial muscles), controlled/opportunistic energy recovery and transfer; and micro active flow control. The research in this area focuses on understanding the interrelations between forms and functions, shapes and behaviors, structures and dynamics, the principles and constraints that govern the interactions between multiple functions, the integration issues that build a coherent functional system based on homogeneous and/or heterogeneous components that have multiple functions, and the adaptive capability allow such systems to dynamically select and switch its functions based on the tasks and environments in hand. Advances in these areas are required to understand and improve the inherent capability of the organic structural components used in military systems and to enhance/enable subsequent applied research in energy harvesting, vibration and noise suppression, prognostics and diagnostics, structural health monitoring, enhanced locomotion and mobility, reduced size/weight/power; increased power density, increased mission functionality and sustainability, and improved articulator manipulation, grasp, sensing, and haptics.

3. Propulsion and Energetics. The goal of this Program Area is explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and our understanding of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area are the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance current understanding of fundamental processes for the development of predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes and the validation of those models. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes, in both gas and condensed phases, and on the peculiarities of combustion behavior in systems of Army interest. To accomplish these goals, the Propulsion and Energetics Program Area has two research Thrusts: (i) Hydrocarbon Combustion, and (ii) Energetics. The goal of the Hydrocarbon Combustion Thrust is to develop kinetic models for heavy hydrocarbon fuels, novel kinetics model reduction methods, surrogate fuel development, and research into sprays and flames, especially ignition in high pressure low temperature environments. In addition the Energetics Thrust focuses on novel material performance via materials design and development and materials characterization, and investigations (theoretical, modeling and experimental) into understanding material sensitivity (thermal and mechanical).

4. Fluid Dynamics. The vast majority of the Army weapon systems involve airborne vehicles and missile systems that are totally immersed in fluids. In turn, the performance of these weapon systems is greatly affected by the resultant forces imparted on them by the surrounding fluid. Consequently, developing highly accurate, stable, agile, and long-endurance weapon systems dictates the need for fluid dynamics research in the areas of interest to both rotorcraft vehicles and tactical missiles. In fact, the battlefield capability and tactical flight operations envisioned for the highly mobile Army of the twenty-first century can only be accomplished through scientific breakthroughs in the field of aerodynamics. Improving performances in every aspects of rotorcraft vehicle performance requires intensive fluid dynamic research in areas, such as, unsteady boundary-layer separation on the suction side of rotorcraft blades, unsteady rotor aerodynamic loads, wakes and interference aerodynamics, and computational fluid mechanics.

Ongoing research topics within this Program Area include the experimental and numerical determination of the flowfield over airfoils undergoing unsteady separation with subsequent dynamic stall, the development of micro-active flow control techniques for rotor download alleviation and dynamic stall control, and the development of advanced rotor free-wake methods to improve predictive capability for helicopter performance, vibration, and noise. To ensure the accuracy and range of unguided gun-launched projectiles and the maneuverability and lethality of guided missiles and rockets, a thorough knowledge of the forces and moments acting during both

launch and free flight is required. These objectives dictate research on shock boundary-layer interactions, compressible turbulence modeling, aft body-plume interactions, vortex shedding at high angle of attack, transonic body flows, and aerodynamic interference effects between various missile components. Examples of current studies in this subfield are the experimental study of aft body-plume-induced separation, and the use of direct numerical simulation, laser-Doppler velocimetry (LDV), and PIV techniques to investigate axisymmetric supersonic power-on/power-off base flows. Research initiatives on the aerodynamics of small unmanned aerial vehicles, both rotary wing and flapping wing, continues. Results indicate that the physics of vortex-dominated flight at low Reynolds number is quite different than that encountered in more familiar high Reynolds number range.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY10 were $24.7 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was $4.8 million. The Division received $5.4 million for allocation to DoD Multi-disciplinary University Research Initiative (MURI), Defense University Research Instrumentation Program (DURIP), and Presidential Early Career Award for Scientists and Engineers (PECASE) programs. In addition, congressional earmarks provided $1.6 million. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided $2.3 million for projects managed by the Division in FY10. Finally, $7.0 million in FY10 was provided by the Defense Advanced Research Projects Agency (DARPA), and $3.8 million was provided by other DoD agencies.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops

1. Multi-Scale Topological Optimization for Next Generation Impact Tolerable Composites (Albuquerque, NM; 29–30 May 2010). The goal of this workshop was to explore promising research approaches needed for identifying the optimal composite plate structure and microstructures for blast resistance using principles of topological optimization. The first full day was a short course geared for Army researchers that focused on topological optimization. The course was taught by Professor Daniel Tortorelli from University of Illinois Urbana-Champaign who is one of the top researchers in the field of topological optimization.

2. Understanding the High Rate Response of Advanced Aluminum Alloys (Baltimore, MD; 3–4 May 2010). The goal of this workshop was to discuss new ideas and new needs in fundamental research related to the performance of aluminum alloys under high rate loading conditions. The role of multiscale experiments and modeling techniques to understand the inelastic mechanisms at the grain and sub-grain level was the primary focus of the workshop. The participants were comprised of researchers from academia, industry and DoD.

3. Intelligent and Adaptive Systems for Dynamic Load Mitigation (Aberdeen, MD; 27-28 May 2010). The purpose of the workshop was to explore the next generation of fundamental research needed for the development of future systems capable of the mitigation of dynamic loads associated with hostile actions. The lectures and discussions explored the appropriate areas of research needed to exploit material design enabling active response to a variety of dynamic loading conditions. The discussed subjects involved novel multi-physics, multi-scale modeling and experimental techniques needed to investigate the physics-based mechanisms that provide an understanding of the role of active constituents in response. A number of novel research areas were recommended (*e.g.*, innovative microstructures, multi-scaled structures, tunable smart devices, and hierarchical nanostructured adaptive materials) that offer directions for future research for the enhancement of blast and penetration resistance of Army structures. Emphasis was placed on the need for "out-of-box" research exploring pioneering, visionary, and possibly controversial ideas that address emerging and future threats.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant

portion of the basic research programs managed by the Division; therefore, all of the division's active MURIs are described in this section.

1. Nano-Engineered Energetic Materials. This MURI began in FY04 and was awarded to a team led by Professor Richard Yetter at the Pennsylvania State University. The objective of this research is to develop the understanding and capabilities needed to engineer multi-dimensional nanoscale energetic materials systems whose energy release can be controlled in terms of its type, rate, spatial distribution, and temporal history. This objective will be achieved through the manipulation of individual atoms and molecules and the control of their assembly into a large-scale bulk energetic material.

The possibility exists to build large-scale energetic materials with a very high degree of uniformity (*i.e.*, few/no defects, perfect crystalline structure, composites with molecularly-engineered uniformity, laminated composites with structures built molecularly, controlled and selectable layers without stirring or mixing) all made possible through self-assembly. It is also possible to embed molecular scale devices within the energetic matrix (embedded smart devices and sensors). Specific topics under investigation are: (i) the development of the chemistry, physics and materials science of nanoscale energetic materials, focusing on those processes that lead to well-ordered structures (*e.g.*, self-assembly, vapor deposition), (ii) computational methods to assess the reactivity of candidate structures and to predict the stability of the energetic material structure, to both hazards (*e.g.*, shock, spark) and to long-term degradation, which will also provide guidance to and receive validation from the experimental aspects of the program, specifically the formulation and characterization activities, and (iii) the development of experimental methods for characterizing nanoenergetic structures to verify structure and performance. This includes development of techniques capable of the determination of the three-dimensional structure of the nanoscale assembly and the orientation and bonding of the constituents. Long-term Army applications include advanced energetic materials with tailored energy release rates.

2. Enabling Science for Future Force Insensitive Munitions. This MURI began in FY05 and was granted to a team led by Professor Don Thompson at the University of Missouri, Columbia. The objective of this MURI is to understand and predict the sensitivity of energetic materials to externally-impressed mechanical and thermal loadings. The specific goals include developing understanding of the chemistry and physics that determine the onset of chemical reaction in crystalline energetic materials and their formulations.

This project is a coordinated effort by several research groups. The first group, headed by Professor Thompson, is developing a unified, multiscale model to predict energetic material sensitivity. The second group, headed by Professor Malcom Nicol of the University of Nevada, Las Vegas, is investigating the effect of defects in energetic crystals upon mechanisms of initiation and energy release. Additional researchers in this effort include Professor William Goddard III at the California Institute of Technology, who is investigating the fundamental chemistry and physics of energetic materials under extreme conditions using the ReaxFF reactive potential. Efforts at developing multi-scale models of the phenomena are by Professor Michael Ortiz, also at the California Institute of Technology. Research from this project is closely monitored by, and coordinated with investigators from DoD and DoE laboratories.

3. Ultrafast Laser Interaction Processes for LIBS and Other Sensing Technologies. This MURI began in FY06 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to develop a theoretical understanding of femtosecond laser/materials interaction that is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations. These models will then be extended to the irradiation of complex sample matrices characteristic of chem/bio threat scenarios, and the use of advanced laser beam modalities, including femtosecond laser self-channeling (FLSC), with an ultimate goal to develop laser induced breakdown spectroscopy (LIBS) stand-off technologies to the kilometer range. This understanding is expressed in combined physical and chemical models, rigorously grounded by experimental characterization and detailed physical and chemical observations relevant to LIBS and other spectroscopic sensing techniques. The techniques include fluorescence, Raman scattering and resonance enhanced multiphoton ionization, (REMPI). The models will then be extended to irradiation of complex material samples characteristic of chemical and biological threat scenarios, as well as energetic materials such as those found in improvised explosive devices (IEDs).

4. Spray and Combustion of Gelled Hypergolic Rocket Propellants. Two MURIs in this topic area began in FY08. One team is led by Professor Stefan Thynell at the Pennsylvania State University, and the second team is led by Professor Stephen Heister at Purdue University. The objective of these MURIs is to understand the processes and mechanisms that control droplet formation, droplet collision and mixing, ignition, and energy release in gelled hypergolic propellants. The projects involve research in the areas of ballistic imaging, aerosol shock tubes, and ultra-fast laser diagnostics to capture reaction characteristics, and focusing on fluid and gas dynamics, chemistry, chemical kinetics and reaction mechanisms, computational fluid dynamics with reactive chemistry, heat transfer, high-performance computing modeling and simulation, and advanced experimental diagnostic methods. The ultimate goal of the efforts is to gain understanding allowing for the science based design of gelled hypergolic propulsion injector and combustor systems. The pursuit of this research may also yield unexpected paths leading to the discovery of new concepts for hypergolic propulsion. The team led by Professor Thynell has developed an integrated research program comprising material science, chemistry, physics, and engineering to address various fundamental issues critical to the development of gelled hypergolic propellant (GHP) spray and combustion technologies for future rocket and missile propulsion systems. New techniques will be developed that will resolve the entire range of length and time scales (from atomistic to device levels). Emphasis will be placed on both microscale and macroscale processes that dictate the propellant interfacial dynamics and chemical initiation mechanisms, as well as the propellant atomization, mixing, and flame development. The team led by Professor Heister is investigating the rheological characterization of gelled propellants, non-Newtonian flow physics of gelled propellants, and combustion physics of gelled hypergols.

D. Small Business Innovation Research (SBIR) – New Starts

Research efforts within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as was discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Cavitation as Traumatic Brain Injury (TBI) Damage Mechanism from Improvised Explosive Device (IED) Blast. A Phase II SBIR contract led by ATR, Inc., is testing the hypothesis that cavitation might be a possible damage mechanism in TBI from blast loading. The project seeks to develop and validate mathematical tools to accurately predict stresses, strains and cavitation from blast, and to develop mitigation technologies that reduce or eliminate damaging effects from cavitation and cavitation/stress-strain combinations. This will be accomplished by leveraging the Navy-developed fluid/structure interactive code, DYSMAS, that is specifically designed to accurately simulate air explosions (AIREX) and underwater explosive (UNDEX) effects and adapt it to the challenging task of simulating the response of the brain to blast. To date, cavitation has not been accurately captured computationally; if successful the knowledge gained from this project will lead to both improved warrior protection and treatment for TBI.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Development of Multi-Layer Aluminum Alloys. A Phase II STTR contract led by Touchstone Research Laboratory is attempting to demonstrate the feasibility of hot roll bonding different aluminum alloys together in order to improve ballistic properties by 20% compared to alloy 2519-T87, while also improving rupture resistance over alloy 5083-H131. In order to identify an optimal combination of layers, the experimental work was aided by computational modeling methods. Processing of multilayer assembly of aluminum alloys includes hot roll-bonding followed by solution heat treatment (SHT) at an appropriate temperature, quenching, cold working, and aging to T8 temper to attain peak strength. The objective of roll-bonding is to develop a metallic bond between atoms across the interfaces of the composite assemblies. If successful the layering approach should improve performance while maintaining or reducing weight.

2. Particle Imaging Velocimetry and Thermometry. A Phase II STTR contract led by ORBETIC, Inc., is attempting to design, develop and demonstrate the feasibility of a flow imaging system that can simultaneously and accurately reveal the spatially correlated flow velocity and temperature fields in at least two dimensions of a reacting, high temperature system. Rare-earth doped nano-crystals whose fluorescence varies as a function of temperature will be used as the seed particles for a conventional system. The fluorescence signal will be used to

measure the temperature of the seed particle, which in turn gives information about the local temperature of the flow. In this manner, information about the velocity and temperature of a turbulent reaction flow (as found in nearly all propulsion systems) can be obtained simultaneously. The information will be critical to validation of design models of various propulsion systems.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

No new starts were initiated in FY10.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Mechanical Sciences Division initiated six new DURIP projects, totaling $0.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of the effects of a shock wave on a single molecule to develop understanding of energetic material initiation, studies to develop new diagnostic techniques to investigate flow separation in unsteady flowfields, and new imaging systems to allow better understanding of damage mechanisms in composite materials.

I. DARPA Reactive Material Structures Program

The Mechanical Sciences Division is serving as the agent for the DARPA-sponsored Reactive Material Structures (RMS) program. This program was initiated late in FY08 with an objective of developing and demonstrating materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Mechanical Sciences Division.

A. Exploring Multi-scale Hierarchical and Topological Structure Design

Professor Markus Buehler, Massachusetts Institute of Technology, Single Investigator Award

The objective of this project is the computational and theoretical analysis of failure mechanisms in hierarchical structures and materials found in biology's structural materials, and the transfer of the results towards the design of hierarchical bioinspired heteronanocomposites. By developing and applying a model that couples atomistic to mesoscopic scales, the major outcomes of this basic research are: a (i) systematic analysis of deformation and failure mechanisms in biological hierarchical structures (such as bone and spider silk), (ii) development of designs for heterogeneous materials involving variations in hierarchical structure and topology for damage tolerance, and (iii) development of a hierarchical transition state based theory (H-TST) capturing deformation mechanisms at multiple hierarchical levels, resulting in hierarchical Ashby deformation mechanism design maps.

A novel element of this project is the use of atomistic-based multi-scale modeling to explore the opportunities and potential of including the atomistic, molecular and mesoscale structure in the engineering design space by an integrated treatment of structure and material. Preliminary progress has been made to formulate a novel mesoscale model to describe the fracture of hierarchical composites and to develop a full atomistic molecular model of a collagen fibril (the basis of bone). Collagen constitutes one third of the human proteome, providing mechanical stability, elasticity and strength to connective tissues. Collagen is also the dominating material in the extracellular matrix (ECM) and is thus crucial for cell differentiation, growth and pathology. However, thus far no atomistic-scale molecular model of collagen fibrils has been reported and fundamental questions remain with respect to the unique mechanical properties of collagenous tissues. By combining x-ray diffraction data with theoretical protein structure prediction methods, Professor Buehler has developed an experimentally validated all-atom collagen microfibril model with full-length molecules, which fully captures key structural features, such as quasi-hexagonal molecular packing and D-banding periodicity (see FIGURE 1).

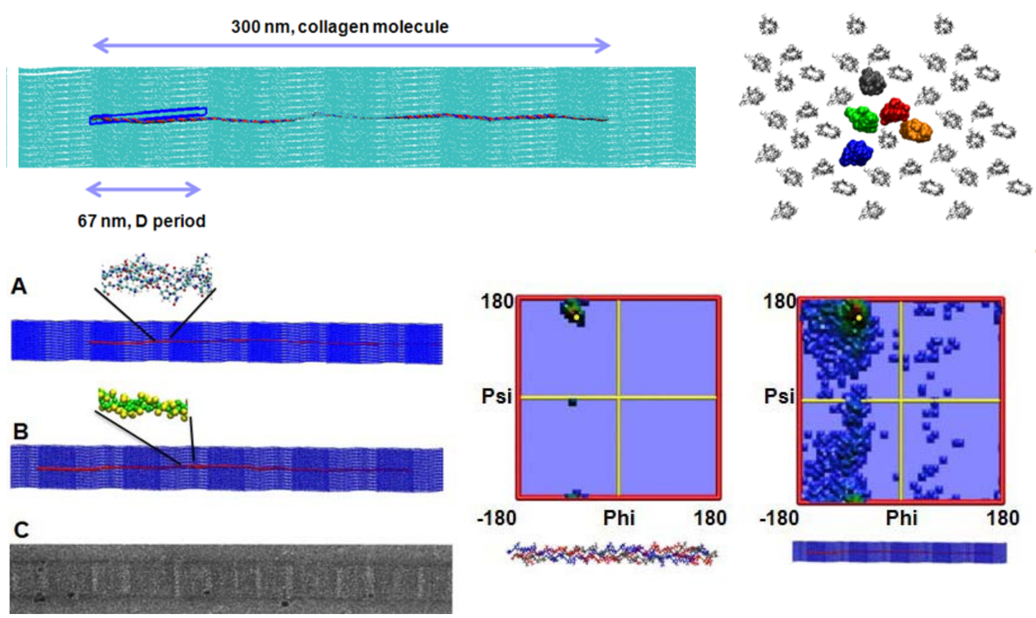


FIGURE 1

The first experimentally-validated model of a collagen fibril. A systematic analysis of the molecular deformation mechanisms reveals that the unique mechanical properties of collagen fibrils can be explained based on their hierarchical structure. The images on the left show the (A) atomistic representation, (B) course grain representation, and (C) photo micrograph representation of the fibrils. The model features key structural features of collagen fibrils, in particular D-banding.

Mechanical testing of hydrated collagen fibrils yields a Young's modulus of ≈300 MPa at small, and ≈750 MPa at larger strains, in excellent agreement with experimental data. Dehydrated collagen fibrils show a significantly tighter molecular packing and increased Young's moduli. Using a systematic analysis of the molecular deformation mechanisms, the PI has demonstrated that the unique mechanical properties of collagen fibrils can be explained based on their hierarchical structure.

A key result of these findings is that deformation is mediated through a series of mechanisms that operate at different hierarchical levels, involving straightening of disordered and helically arranged molecules at small strains followed by axial stretching and molecular uncoiling. This explains the striking difference of the modulus of collagen fibrils compared to single molecules, which exceeds 4 GPa, (10-20 times greater). These findings substantiate the notion that collagen tissue properties are extremely scale dependent. A key impact of this work is that the atomistic model of collagen fibrils now enables the bottom-up elucidation of structure-property relationships in a broader class of materials.

B. Exploring Hierarchical Engineered Materials and Structures
Professor Anthony M. Waas, University of Michigan, Single Investigator Award

The objective of this project is to develop a comprehensive understanding of the deformation response and failure of multimaterial structures at high rates of loading using a combination of experiments, analysis and computational modeling. To this end, the investigator is exploring how stiffness, strength, energy absorption and damage growth can be controlled by tailoring a material's microstructure. The research is establishing new high rate test procedures to measure how multimaterials deform in real time and the investigator is using this information to develop advanced computational models that capture physics of failure.

This research may reveal how deformation coupling mechanisms can be exploited in the design of material architecture. This research has resulted in the first experimental measurements to capture the *full-field* deformation response of complex multimaterials such as 3D textiles and honeycombs under high loading rates and under multi-axial stress states (see FIGURE 2). The research is relevant to a multitude of infrastructure and vehicle applications including protective materials.

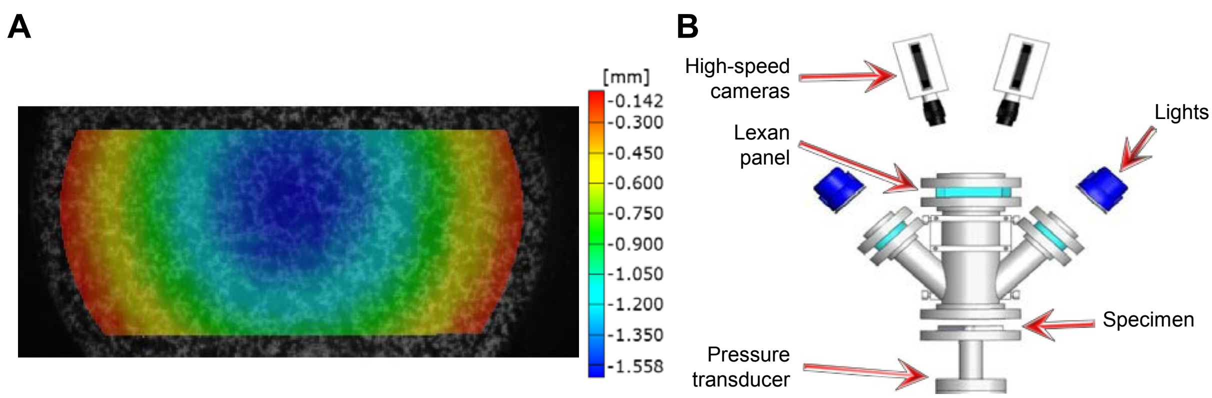


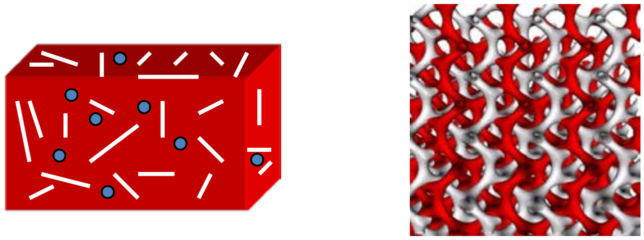
FIGURE 2

Unique test and measurement scheme of real-time deformation fields and failure mechanisms. This measurement scheme enables measurement of the full-field deformation response of complex multimaterials, such as 3D textiles and honeycombs, under high loading rates and under multi-axial stress states.

C. Failure Characterization and Modeling of Lightweight Interpenetrating Network Composites
Professor Hareesh Tippur, Auburn University, Single Investigator Award

The objective of this project is to gain fundamental insights and in-depth understanding about how the behavior of interpenetrating phase composites (IPC) is governed by its microstructure. Novel interrogation methods are being developed for the failure characterization of IPC foam systems involving open-cell metallic scaffolds infiltrated by lightweight polymer syntactic. Unlike conventional composites, the constituent phases in these composites are interconnected three-dimensionally and topologically throughout the microstructure; that is, both matrix and reinforcement phases interpenetrate throughout the microstructure in all the three spatial dimensions

(see FIGURE 3). Consequently, the architecture of an IPC helps each phase to contribute its property synergistically to the overall macro-scale characteristics. IPC architecture also enables tailoring residual stresses in the constituents of the composite to produce an advantageous macro scale response.



Traditional composite Interpenetrating phase composite

FIGURE 3

Traditional composite versus interpenetrating phase composite (IPC). The architecture of an IPC helps each phase to contribute its property synergistically to the overall macro-scale characteristics.

In this research, a combination of global and local mechanical measurements are being made using full-field optical methods for understanding the failure behavior of the constituent phases as well as the composite foam. Complementary finite element modeling is being used to augment experimentation. Currently, material responses from low and high strain rate conditions are being compared in order to identify loading rate effects. Quasi-static compression tests have been performed on cylindrical Syntactic Foam (SF) and IPC samples. The plateau stresses for IPC foams are greater than the sum of the plateau stresses of the corresponding SF and unfilled aluminum preform/scaffold. This is attributed to the prevalence of synergistic constraint between the scaffold and SF phases of the 3D interpenetrating microstructure. The energy absorbed up to 22% true strain for SF and IPC samples show that IPC absorbs ~35% higher energy per unit volume than the corresponding SF under quasi-static conditions. IPC also outperforms SF samples by 10-15% when energy per unit mass is a consideration. A split Hopkinson pressure bar apparatus has been developed and calibrated for testing low-impedance materials at strain rates of ~1,600/sec. Cylindrical SF and IPC foam samples have been prepared and dynamic compression testing has been carried out. The results show that under dynamic loading conditions, SF and IPC samples show a stress-strain response that has only two dominant regimes – a linear zone up to a maximum stress, and a monotonically softening zone that follows. The foams with lower volume fraction (V_f) of microballoons tend to soften more rapidly than the ones with higher V_f. The maximum stress increases with decreasing V_f for microballoons under high-strain rate conditions. The values for IPC foams are again 10-15% higher than those for SF under dynamic conditions. The dynamic maximum stress values are also higher for both SF and IPC relative to the quasi-static ones. The failure modes and mechanisms have been characterized using high-speed photography of linear grating patterns printed on the specimen surface during compression failure in split-Hopkinson pressure bar. Unlike in quasi-static loading conditions, high-speed optical recordings reveal significant spring-back in syntactic foam whereas it is negligible in IPC foams.

D. Exploring Passive and Active Mechanisms of Massively Separated High-Speed Flow Control

Professors J. Dutton and G. Elliott, University of Illinois, Urbana-Champaign, Single Investigator Award

The objective of this project is to study flow-control methodologies and potential effects on high-speed separated flows. The flow fields of interest to this research include missile and projectile base flows. The expected outcomes are to further the basic understanding of these complex flow fields and to effect substantial changes in these base flows that will lead to improved flight vehicle performance.

The investigator successfully completed passive flow-control experiments by inserting triangular splitter plates into the recirculation region behind the cylindrical base to alter the stability characteristics and flow structure of the near-wake flowfield. Schlieren photography, surface flow visualization, mean static pressure measurements, and pressure-sensitive paint (PSP) measurements were successfully performed to characterize the effects of the passive flow-control splitter plates. Active flow-control experiments are currently underway. In addition, a number of active flow-control actuators are being researched for potential base flow experiment applications. Potential actuators include: (i) implementing the current plasma actuator infrastructure to power plasma

synthetic jet forcing of the shear layer, (ii) applying dielectric barrier discharge actuators on the afterbody, and/or (iii) exercising piezoelectric actuators at high frequencies to disrupt or incite the azimuthal instability modes of the separating flow. The electric-arc plasma actuator was successfully designed and constructed, and waveforms of the voltage and current, emission imaging, Schlieren imaging, spectroscopy, and preliminary particle image velocimetry (PIV) data have all been acquired for the base case of the actuator in quiescent air (see FIGURE 4).

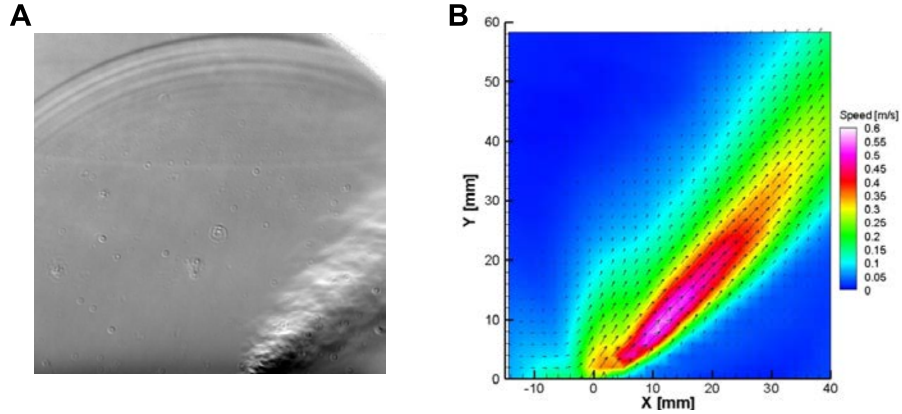


FIGURE 4

Flow control approaches. Figure (**A**) shows Schlieren images of the electric-arc plasma actuator and (**B**) is the averaged velocity field at 40 μs after plasma emission for the electric-arc plasma discharge in quiescent air while mounted in a recessed cavity in a piece of boron nitride at 45-degrees inclination.

E. A Study of Supersonic Compression Corner Interactions Using Hybrid LES/RANS Models

Professor Jack Edwards, North Carolina State University, Single Investigator Award

The objective of this research is to develop a new class of hybrid turbulence modeling strategies that use Reynolds-averaged Navier-stokes (RANS) concepts to model the inner part of a turbulent boundary layer while modeling most of the boundary layer as a large-eddy simulation (LES). This strategy significantly reduces the mesh resolution necessary to capture the dominant turbulent eddies, paving the way for practical LES calculations of high speed flows of interest to the Army. This model differs from existing models in the literature in that the transition modeling concept from RANS to LES is not considered to be a function of the mesh resolution, but rather a function of the boundary layer structure. Consequently as the boundary layer shifts from its near-wall logarithmic behavior to its wake-like structure, the current model transitions from RANS to LES. In addition this model is sensitive to other flow field features and allows for the proper adjustments from boundary-layer equilibrium, as induced by shock waves and other mechanisms that allow for strong departures. The model development and validation efforts were carried out on the flow field simulations of the flat-plate turbulent boundary layers at different conditions (see FIGURE 5).

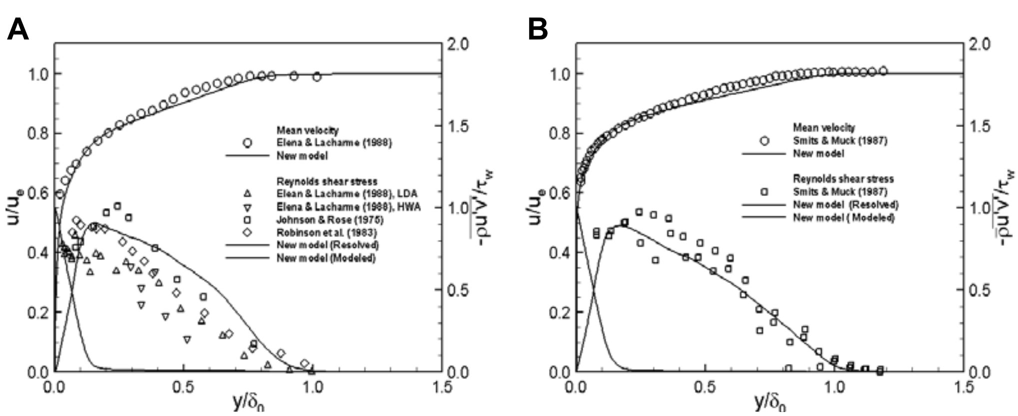


FIGURE 5

Boundary layer velocity and Reynolds shear stress predictions. Results of (**A**) velocity and (**B**) Reynolds stress profiles within the boundary layer are shown, as predicted by the current model, and compared to other well established models.

Currently research efforts are underway to use these techniques to simulate an array of benchmark experiments involving shock wave/turbulent boundary layer interactions that were mapped at Princeton University from 1978-1994. If successful this effort will provide a high-fidelity modeling approach that will directly capture most of the unsteady physics associated with boundary layer interactions and thus leads to the accurate prediction of forces, moments, and heating loads on surfaces immersed in fluids. In addition the current LES/RANS model is significantly less expensive than wall-resolved LES or direct numerical simulation. This means that it can be applied without simplification to flow fields of interest to the Army.

F. Multifunctional Carbon Nanotube-Based Composites Tailoring for Structural Damping

Professor Charles Bakis, Penn State University, and Professor Kon-Well Wang, University of Michigan, Single Investigator Awards

The objective of this research is to advance the state of the art of structural damping by exploring the fundamental mechanisms of damping provided by carbon nanotubes (CNTs) in polymer-based materials used to fabricate fiber composites, and to use the results to explore further enhancements in damping. The feasibility of using carbon nanotubes for damage detection in polymeric composites is also being explored.

Multi-scale micromechanics - molecular dynamics models of CNTs embedded in polymer resin - have been developed to simulate damping of aligned and unaligned CNTs. The models point to the importance of CNT morphology and functionalization in overall damping behavior of the composite. Using the models epoxy resin containing well dispersed, aligned or randomly oriented functionalized SWNT ropes are investigated. The molecular dynamics analysis indicates that the interfacial shear strength between the SWNT and the epoxy resin is dependent on different quantities of functional groups on the CNT. With about 1% carbon atoms in the CNT covalently bonded to the epoxy resin, the interfacial shear strength is about 25 times the value for non-functionalized CNTs in epoxy. The effective loss factor for the epoxy resin with functionalized CNTs are investigated and compared with the epoxy resin containing non-functionalized CNTs (see FIGURE 6). With functionalized CNTs, the onset and completion of the interfacial slip occurs at higher cyclic (tension-compression) stress amplitude, although the maximum loss factor does not change. Functionalization can either enhance or reduce damping based on the interfacial shear strength and the operational stress range of the chosen matrix material. Regarding the randomly oriented case examined in this investigation, the functionalization of CNTs reduces the effective loss factor if the operational stress range is low. However functionalization can enhance damping if the operational stress range is high. The investigators concluded that with well-dispersed and well-tailored CNTs, the structural damping capability of composites can be increased significantly.

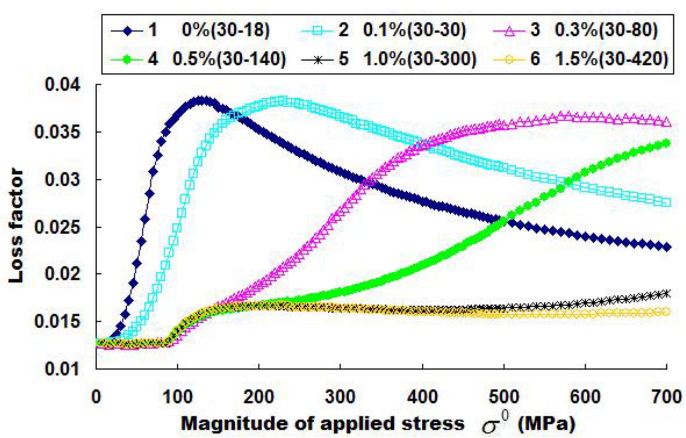


FIGURE 6

Loss factor of epoxy composite with in-plane, randomly oriented functionalized SWNT ropes under tension-compression cyclic loading. The legend indicates the case number, the CNT functionalization scale, and the corresponding two interfacial shear strengths at the inter-tube and CNT/epoxy interface. For instance, "1 0% (30-18)" represents Case 1 for a composite with non-functionalized CNTs, which has an inter-tube shear strength of 30 MPa and CNT/epoxy shear strength of 18 MPa.

Following the predictions of multi-scale modeling and analysis on the effects of CNT volume fraction and CNT aspect ratio on damping, it is desired to manufacture damping composites with higher weight fractions of long CNTs that are aligned in the direction of loading. Therefore novel methods of aligning and chaining carbon nanofibers and CNTs with AC electric fields have been developed and used to make epoxy-based composites. Multiphysics models of CNT chain formation in liquid epoxy explain the experimental observations of peak chain growth at a certain optimal electrical frequency. The research result also indicated that a damage crack in a CNT-based composite could be detected with significantly greater sensitivity if external tuned resonance circuitry is used.

Applications of this research exist for the Army in stability augmentation, vibration control, and health monitoring of rotorcraft, weapon systems, and military vehicles. This will result in system performance improvement, life extension, cost reduction, and enemy detection prevention. Discussions between the investigator and ARL-WMRD revealed that his effort can greatly benefit ARL research on lightweight composite structures for weapons systems.

G. Damage Characterization, Structural Health Monitoring and Residual Life Prediction of Composites
Professor Aditi Chattopadhyay, Arizona State University, Single Investigator Award

The goal of this research is to characterize damage and structural health monitoring (SHM) of composite structures. To assess the physical condition of critical structural components, a major challenge is scaling material and structural behavior across different length scales in order to model full-scale structural response and damage evolution. It is important to optimally integrate sensory devices to enhance structural performance and reliability of the monitoring system. This research addresses two key elements in a SHM framework - material characterization and constitutive modeling, and sensor systems. The development of an accurate multiscale modeling approach will depend on the use of proper constitutive models of the constituents.

This research is being completed with the assistance of Professors M. Fard, and C. Hiche at Arizona State University, and is focused on the nonlinear behavior of polymer matrix materials under flexural loading. Experimental results obtained from a digital imaging correlation (DIC) system captured some of the fundamental features of the tensile and compressive true stress strain behavior of epoxy resin materials. Experiments on cubic, prismatic, and cylindrical compression samples were performed and showed that strain stiffening at high strain values in the cubic samples is due to barrel-like phenomenon and triaxial stress state. Therefore for large strain values, strain hardening can be ignored in the constitutive behavior (see FIGURE 7).

A novel analytical technique has been developed for epoxy resin materials to investigate the effects of out-of-plane loading on the constitutive relationship based on two different stress strain models. The first is a strain softening model for tension and compression defined by 14 unique parameters. The second model is a simplified constitutive law with constant plastic flow in tension and constant yield in compression defined by 11 unique parameters. A complete set of analytical parametric studies, based on the developed closed-form solutions for moment curvature response and numerical simulation of load deflection response, show the correlation of flexural load carrying capacity of epoxy resin to different parts of the tension and compression stress strain curve (see FIGURE 8). These results provide insight into improved modeling and design of composite structures to account for the effects of out-of-plane loading. The modified stress-strain relationship based on back calculation of bending tests could be used as an input material model for impact analysis.

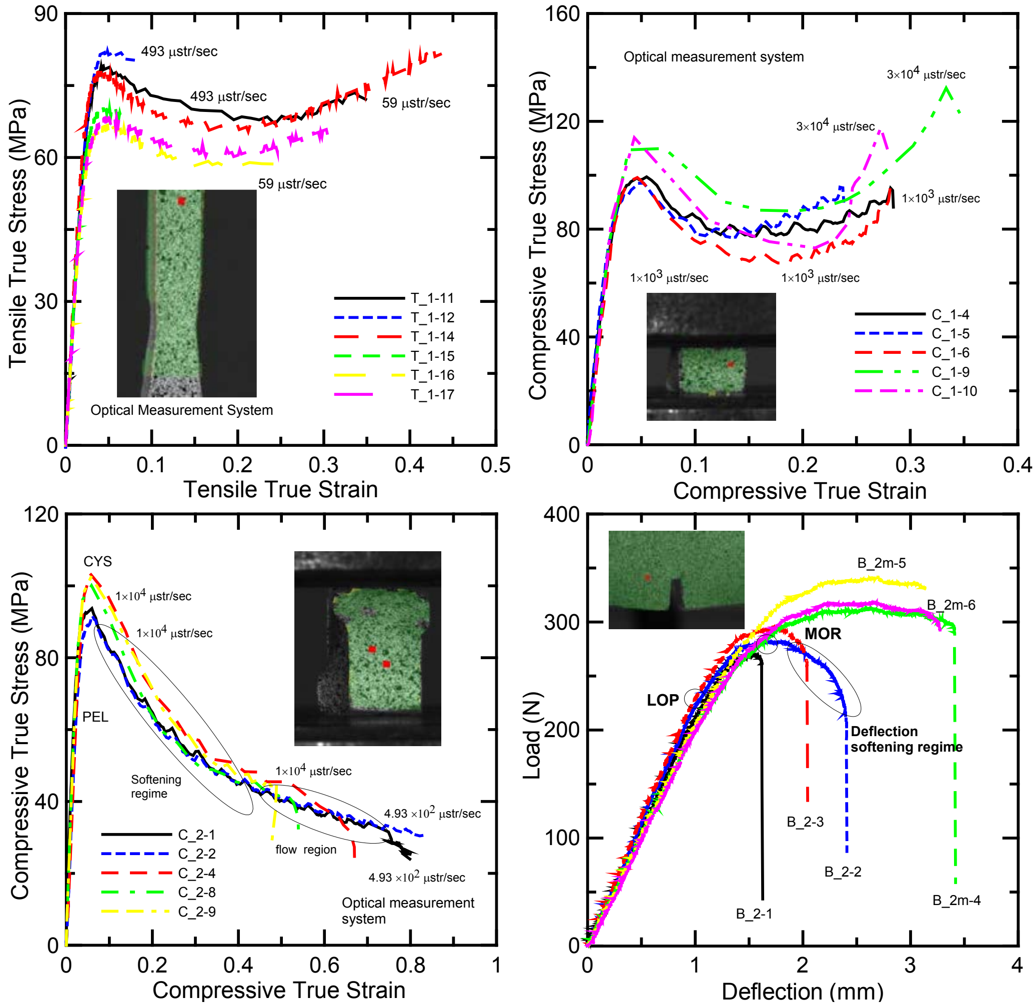


FIGURE 7

Dogbone tensile, cubic and prismatic compressive stress strain and 3PB load deflection responses at different loading rates for epoxy resin Epon E 863. Limit of proportionality (LOP) stress is around 72% of Modulus of Rupture (MOR) stress in out-of-plane loading, while the proportional elastic limit (PEL) stress in tension and compression stress strain curve is around 60% of the stress at the peak points indicating one of the effects of stress gradient in material response.

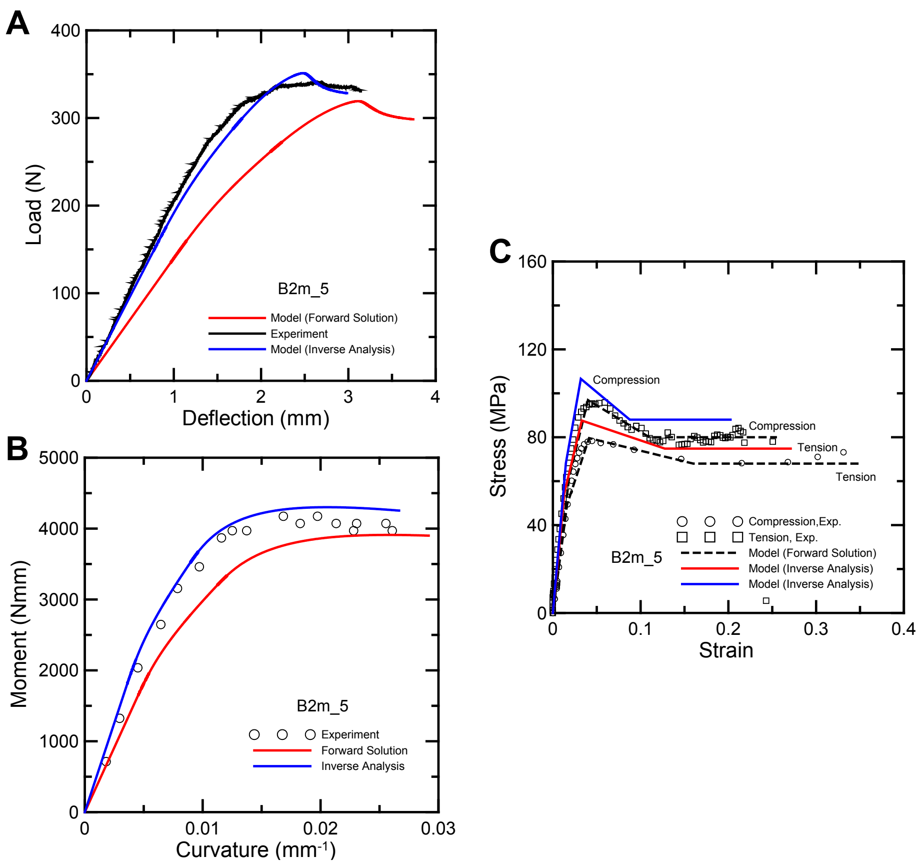


FIGURE 8

Analytical parametric studies show the correlation of flexural load carrying capacity of epoxy resin with different parts of the tension and compression stress strain curve. The data plots show results of (**A**) simulation of load deflection, (**B**) moment curvature response, and (**C**) the back calculated stress strain response. Forward solution and inverse analysis technique for epoxy resin flexural specimens showed that the direct use of the tension compression stress strain model under-predicts the moment curvature and load deflection responses.

A fast and efficient localization algorithm was also developed for impact damage on composite plates that shows good correlation with experimental data (see FIGURE 9). These results demonstrate the feasibility of implementing this inexpensive methodology for accurate impact localization in complex composite structures.

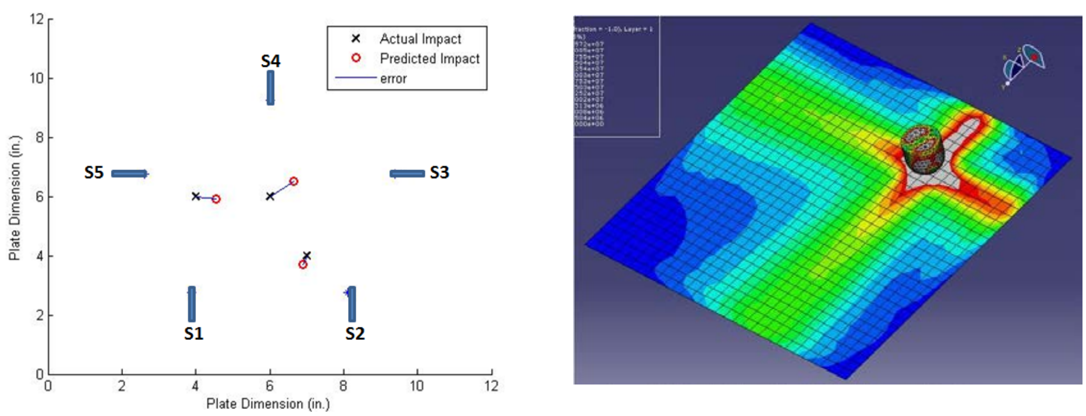


FIGURE 9

Localization results using experimental data from composite plates. The predicted location shows good accuracy with an average error of 0.57in.

Accurate damage localization and characterization of advanced composites would allow performing real-time health monitoring on different Army components, such as motor casings, missile launch tubes, vehicle armor, and ceramic body armor. Low velocity impact damage on motor casings is caused during the mishandling and transportation of weaponry, which can result in more than a 50% reduction in the burst strength, causing accidental in-field impacts. Multi-scale modeling based on accurate material characterization will result in safer and optimal design of composite structures. Therefore a robust SHM framework, which integrates physics-based material models with accurate and efficient damage state awareness techniques, can result in reduced operational cost and minimize accidents. Fiber Bragg Grating (FBG) sensors are used for impact damage identification in woven composite structures. The low weight, small diameter, and multiplexing capabilities of FBG sensors makes them ideal for embedding in composite structural components. Composite helicopter rotor blades and vehicle armor, such as in HMMWV's, could be monitored in real-time to assess the integrity of the panels to avoid accidents and casualties. Furthermore if combined with a prognosis framework, it could predict the useful life of the panels, reducing the operational costs and downtime of the vehicles.

H. Combustion and Ignition Studies of Nanocomposite Energetic Materials

Professor Michelle Pantoya, Texas Technical University, PECASE Award

The goal of this project is to understand the processes controlling extraction and conversion of stored chemical energy to develop an understanding of combustion behaviors of energetic composite materials (*i.e.*, reactive materials and thermites) and their role in weapon systems. New diagnostic techniques are also being developed to quantify energy storage and transport under multiple spatial and temporal resolutions. This research addresses questions that fall into four fundamental basic science categories: analytical modeling, experimental investigations, equilibrium kinetics, and diagnostic development.

In FY10 progress towards these overall objectives was made on several fronts. Examination of various time points relevant to reaction propagation reveals that Al particles below 3 nm in diameter evaporate before chemical reactions occur. Because Al particles >> 3 nm in diameter are frequently used, a diffusion flame model was developed to understand single Al particle combustion relative to macroscopic propagation rates. The diffusion flame model predicted orders of magnitude slower propagation than was experimentally observed. These results imply (1) another reaction mechanism is responsible for promoting propagation (such as detonations), and/or (2) other modes of energy transfer play a more dominant role in propagation.

A laser flash analyzer (LFA) was engineered to measure the thermal diffusivity (α) ranging from loose powder to highly consolidated pellets. The measurements can be made from ambient up to 300°C and they are further modifying the system to measure up to 1,600°C. Early results on Al+Teflon reveal that small quantities of graphene will increase the composites thermal properties by 80%. Results with $Al+Fe_2O_3$ show that the heating cycle significantly influences α. Specifically when a composite is exposed to temperatures of up to 300°C then allowed to cool, the mixture exhibits a roughly 30% increase in α.

Experiments to understand the response to mechanical initiation as a function of the composite's compositional and bulk density were performed. Composites ranged in compositional density from 3.5 to 17.9 g/cc and included Al-Ti, Al-Ni, Al-W, Al-Hf, Al-Zn pressed to bulk densities that ranged from 50 to 80% of the theoretical maximum. Al particle size was also investigated and ranged from nm to microns. Results show that the nano Al particle composites are more sensitive to impact ignition than their micron scale counterparts. As bulk density increases, the samples become increasingly sensitive to ignition and display an average 70% decrease in ignition energy. Compositional density also plays a critical role in ignition energy. As the density of the composite increases, regardless of the Al particle size, the composites become more sensitive to ignition. Results show that at the same bulk density, higher compositional density composites such as Al-W require 80% less ignition energy than lower compositional density composites such as Al-Ti.

Energy transfer from reacting thermite placed on a v-notch steel target was evaluated for two thermite compositions: B- Fe_2O_3 and Al-Fe_2O_3. A high speed infrared camera captured the thermal history on the substrate as the reaction propagated. Results quantified the percent of the overall energy available from the chemical reaction that was transferred into the substrate and lost via other heat transfer modes. The B-Fe_2O_3 reaction transferred 53% of its heat of reaction into the steel substrate compared to 11% for Al- Fe_2O_3.

The reaction kinetics of Al and Teflon were investigated using nanoparticles of both. Results showed a unique pre-ignition reaction (PIR) associated with the nano-Al/Teflon mixture that was not significant in the micron-Al/Teflon mixture. The PIR is caused by fluorination of the alumina (Al_2O_3) shell and reduces the onset temperature of Al ignition for nano compared with micron particle mixtures. DSC analysis show reaction kinetics vary dramatically as the alumina particle size is reduced. Specifically smaller diameter alumina particles spur the decomposition of Teflon at lower temperatures. This is a novel approach for manipulating the decomposition properties of a fluoropolymer.

A thermite spray gun was developed for discharging the reaction products and intermediates of the highly exothermic reaction. The thermite spray gun was inspired by more widely used hydrocarbon spray guns with the modification that the reactants are in the solid phase. This device was used in conjunction with a heat flux sensor to examine the energy transfer characteristics of the spray. FIGURE 10 illustrates that micron composites produce a jet capable of target penetration while nano composites produce an aerosolized spray.

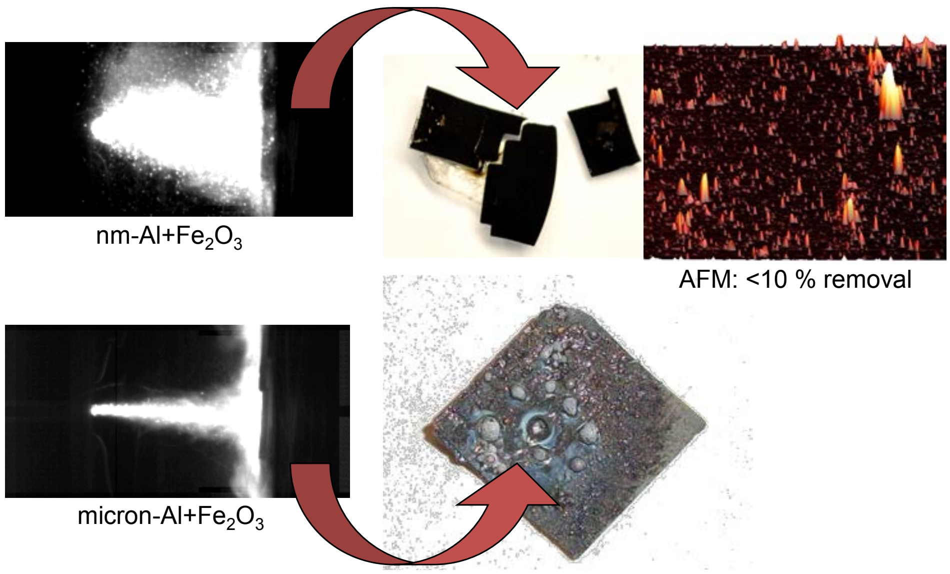


FIGURE 10

Nano versus micron particle formation. These images illustrate the dramatic difference in spray resulting from nano versus micron particle formulation. Images show that micron formulations produce a steady stream of energy capable of penetrating a surface, while nano formulations produce a more dispersed spray that results in removal of less than 10% of the surface.

I. Exploring Autoignition and Combustion of JP-8 and its Surrogates at Moderate Pressures

Professor Kal Sehshadri, University of California, San Diego, Single Investigator and DURIP Awards

The objective of this research is to develop surrogates that can reproduce selected aspects of combustion of JP-8 fuel in laminar non-uniform flows. They include critical conditions of extinction and autoignition, and flame structure. Non-premixed and premixed combustion are considered. The studies are being carried out for values of pressure up to 25 bar. The specific goals are to determine (i) which surrogate best reproduces selected combustion characteristics of JP-8 at atmospheric and moderate pressure, and (ii) the chemical kinetic mechanisms for these surrogates.

Experimental and kinetic modeling studies are in progress and are being carried out employing the counterflow configuration. Fuels tested are JP-8, potential surrogates of JP-8, and reference components. Measurements include critical conditions of extinction and autoignition, and flame structure. Kinetic modeling is carried out using a semi-detailed mechanism. The results are used to validate the chemical-kinetic mechanisms. At present these studies have been carried out at atmospheric pressure. They will be extended to moderate pressures up to 25 bar. It has been established that a useful method to model the combustion of commercial fuels is by developing surrogates. In a previous experimental study supported by ARO, several batches of JP-8, Jet-A, and fifteen possible surrogates of jet fuels, were tested in non-premixed systems. It was found that critical conditions of extinction and autoignition of all batches of JP-8 and Jet-A are similar. Among the surrogates tested, a

surrogate made up of n-decane (80%) and trimethylbenzene (20%) by weight, called the Aachen surrogate, and a surrogate, referred to here as surrogate C, made up n-dodecane (57%), methylcyclohexane (21%), and o-xylene (22%) by weight, were found to best reproduce autoignition and extinction characteristics of JP-8. Kinetic modeling studies were carried out to predict extinction and autoignition for non-premixed combustion of the Aachen surrogate and surrogate C and the results agreeed well with experimental data. Thus the Aachen surrogate and surrogate C accurately reproduce key aspects of JP-8 combustion in laminar non-premixed flows.

Motivated by the success of the Aachen surrogate and surrogate C in reproducing key aspects of combustion of jet fuels in laminar non-premixed flows, these surrogates and a jet fuel were tested in premixed, nonuniform flows. This part of the research was performed in collaboration with scientists at Politecnico di Milano, Italy. In addition to testing the surrogates, the reference components tested were n-heptane, n-decane, n-dodecane, methylcyclohexane, trimethylbenzene, and o-xylene. The counterflow configuration was employed. Studies were carried out by injecting a premixed reactant stream made up of prevaporized fuel, oxygen and nitrogen from one duct, and an inert-gas stream of N_2 from the other duct. Critical conditions of extinction were measured. Experimental data show that the extinction characteristics of n-heptane, n-decane, n-dodecane and methylcyclohexane are similar, as are o-xylene and trimethylbenzene. It was noteworthy that the extinction characteristics of Aachen surrogate and surrogate C were found to be similar to that of JP-8. Flame structure and critical conditions of extinction were predicted for the reference components and the surrogates using a semi-detailed kinetic model. The predicted values were found to agree well with experimental data. Sensitivity analysis shows that the lower reactivity of the aromatic species arises from the formation of resonantly stabilized radicals. These radicals are found to have a scavenging effect. The present study on premixed flows together with previous studies on non-premixed flows show that the Aachen surrogate and surrogate C accurately reproduce many aspects of premixed and non-premixed combustion of fuels.

Experiments were conducted on non-premixed n-decane flames because it is a component of the Aachen surrogate. The fuel stream was a mixture of pre-vaporized fuel and nitrogen and the oxidizer stream was air. Critical conditions of extinction were measured. Concentration profiles of H_2, O_2, CO_2, H_2O, CO, CH_4, and hydrocarbons from C2 to C6 were measured using a gas chromatograph. Temperature profiles were measured using a thermocouple. Kinetic modeling was performed using detailed kinetic models developed by collaborators in Italy. The predicted values of the critical conditions of extinction and autoignition for n-decane agree well with experimental data. The flame structure calculated using the semi-detailed mechanism also agreed well with experimental data. There are however, differences between the predicted and measured mass fraction of those species that have more than three carbon atoms. A "High Pressure Combustion Experimental Facility" (HPCEF) has been constructed for carrying out experiments at pressures up to 25 bar. This facility will be used to study combustion of high molecular weight hydrocarbon fuels in laminar nonuniform flows. In the HPCEF different types of counterflow burners can be placed inside a high pressure chamber. A counterflow burner that can be used to carry out experiments on gaseous fuels has been built and tested at up to a pressure of 6 bar. The facility and a sample burner flame under investigation are shown in FIGURES 11-12.

FIGURE 11

High pressure combustion experimental facility (HPCEF). The photo shows the stainless steel pressure chamber mounted to an aluminum stand, with flanges connecting the cylindrical part to bottom and top reinforced with gussets. The top and cylindrical portions of the chamber can therefore be lifted off without dismantling any connections, and the chamber is enclosed in a high-impact polycarbonate cubicle that provides an additional degree of safety in case of malfunction or accident. Counterflow burners are inside the pressure chamber.

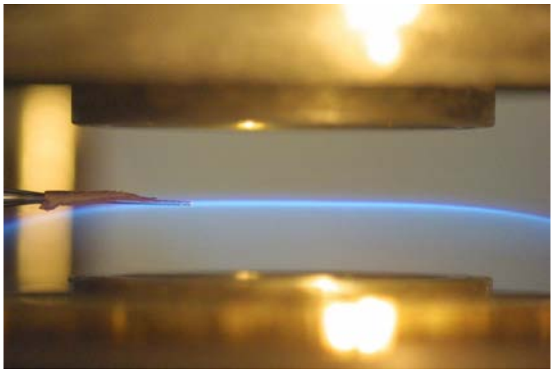


FIGURE 12

Non-premixed n-decane/air flame stabilized in the counterflow configuration. The mass fraction of fuel in the fuel stream is 0.306, the temperature of the fuel stream is 400 K, the temperature of air is 298 K, and the strain rate is 100 s^{-1}. The photo shows the quartz microprobe removing samples from the flame. The samples are analyzed in a gas chromatograph. Note that the quartz microprobe does not disturb the flow-field.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Cell and Tissue Level Mechanisms of Blast-induced Mild Traumatic Brain Injury (mTBI)

Investigator: Raul Radovitzky, MIT, Single Investigator Award
Recipients: Program Executive Office (PEO) Soldier and U.S. Army Aeromedical Research Laboratory

The objective of this research is to identify and understand the mechanisms that cause blast-induced mild Traumatic Brain Injury (mTBI). Using experimental and computational studies spanning the cellular to tissue levels, researchers have been probing the root causes for cognitive deficits resulting from fast rise time, short duration pressure profiles as seen in blast scenarios. One result of this project is the most extensive finite element model of the human head in existence. The model includes eleven different anatomical structures reconstructed from high-resolution 3D magnetic resonance imaging (MRI) data. This head model has transferred to PEO Soldier for the evaluation of new helmet designs and to compare new designs to the current Advanced Combat Helmet. The Army Aeromedical Research Laboratory is also using the head model to evaluate blast sensor technologies for future helmets.

B. Microstructurally Engineered Materials

Investigator: Mohammed Zikry, North Carolina State University, Single Investigator Award
Recipient: ARL-WMRD

This project focuses on the optimization and development of a new class of high strength and lightweight aluminum alloys for armored systems subjected to high rate and severe loading conditions associated with IED events. The effort utilizes an integrated experimental and atomistic and microstructural modeling framework to rapidly identify dominant microstructural material characteristics. These results have been used to significantly improve ballistic response through tailored processing for desired applications. The project has already led to a new state-of-the-art in the aluminum armor alloy technology. The ultimate goal is to develop very high mass efficiency aluminum armor alloys that are resistant to blast and penetrative events. This research is providing a critical link between macroscopic dynamic response, microstructural characteristics, and inelastic mechanisms at relevant length and time scales. This basic research has transitioned to ARL-WMRD where it is being used to enrich parallel applied research efforts and help develop new and significantly improved armor designs.

C. Condensed Phase Product Penetration and Flame Spreading Processes in Granular Bed

Researcher: Ken Kuo, Pennsylvania State University, Single Investigator Award
Recipients: ARL-WMRD, Army Armament Research, Development and Engineering Center (ARDEC)

The objective of this effort was to develop fundamental information about the ignition and flame spreading behavior of granular propellant beds to enhance understanding and to facilitate the predictive capability of the codes. Specific goals of the work were to measure the condensed-phase product penetration from an igniter jet into a granular propellant bed, find the flame-spreading rate in the granular bed as a function of different igniter jet configurations and geometries, and determine the effect of vent-hole pattern on igniter jet penetration depth and associated energy transfer rates on granular propellant ignition and combustion processes. The results of this project were shared with many ARL researchers, including Dr. Mike Nusca, Dr. Dick Beyer, Dr. John Schmidt, Dr. Tony Kutler, Dr. Lang-Mann Chang, and Dr. Stephen Howard with highly positive feedback. Results were also shared with many individuals at ARDEC, and these data will also be used to validate codes for the prediction of mortar internal ballistics.

D. Nonlinear Signal Processing of Standing and Traveling Waves for Diagnosis and Prognosis of Filament Wound Components Subject to Combined Loads
Researcher: Douglas Adams, Purdue University, Single Investigator Award
Recipients: Aviation and Missile Command's Condition-based Operations and Sustainment Technology Aviation (COSTA) program; Sikorsky Aircraft Corp.

The objective of this project was to quantify how applied multi-loading sequences consisting of inadvertent impacts, temperature cycles, moisture, and ultra-violet radiation can lead to changes in material response, degradation, and damage accumulation in filament wound components. Based on their research, the investigators developed a process capable of quantifying an impact and its location while in operation with the potential to greatly reduce resources committed to inspection (see FIGURE 13). As a direct result of published results, Sikorsky has sub-contracted to Purdue for the recently awarded COSTA program to develop an impact force identification algorithm for composite helicopter blades using minimal sensing to identify damaging loads.

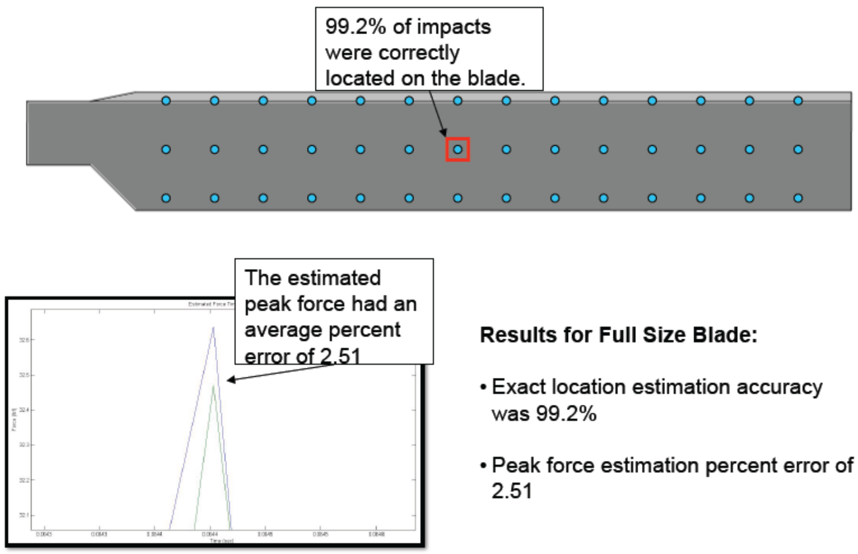


FIGURE 13

Results of impact localization testing on helicopter blades. Using the method developed at Purdue University, an impact and its location can be quantified while in operation, providing a significant reduction in the resources committed to inspection.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Novel Actuation and Control of Highly Articulated Mechanisms

Professor Howie Choset, Carnegie Mellon University

Highly articulated mechanisms can extend the classic six-degree-of-freedom robotic manipulator into the realm of tens, hundreds, or even infinite degrees of freedom with a promise of increased functionality through multiple kinematic solutions and restricted-space navigation. For example, snake robots may be able to thread through tightly-packed volumes and access locations that people and machinery otherwise cannot access and can do so with minimal invasion. However these highly-articulated mechanisms also come with significant challenges and complexities in terms of inverse-kinematic and control calculations, mechanism collision avoidance, multiple-kinematic-solution selection and optimization, and sufficient joint strength and power/weight ratios. Previously, the investigators constructed a small surgical robot for minimally-invasive cardiac surgery (see FIGURE 14). This new, jointly-funded ARO/TATRC research effort takes a two-tiered approach to advancing the state of the art.

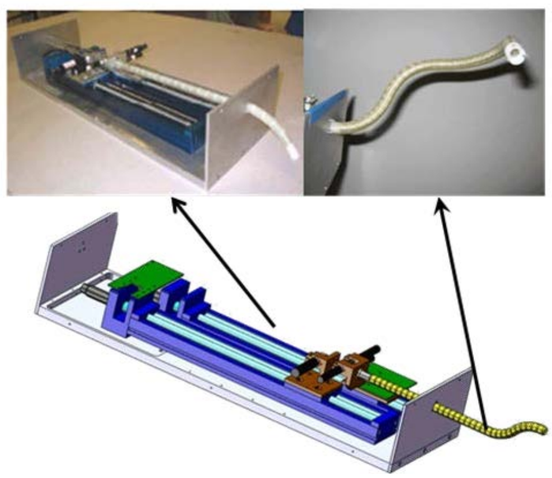


FIGURE 14

Surgical snake robot. It is anticipated that the current research will lead to the identification of the feature sets required to improve the previously-developed snake robots with extended lengths and improved force-feedback control

It is anticipated that this research will lead to identification of the feature sets required to improve the previously-developed snake robots with extended lengths and improved force-feedback control. This project aims, in the long term, to enable technologies such as mechanism design and closed feedback control of highly-articulated serpentine robots. Currently, design methodologies that consider tradeoffs among actuation, link materials, and force delivery do not exist. As such the research seeks to develop a novel framework to consider these issues. It is envisioned that a serpentine arm may be used in conjunction with an automated guided vehicle (AGV) or robot arm. Hence, the integration of the serpentine mechanism and control with the AGV or arm must also be considered. Finally, the serpentine system will perform a task, whether it is cutting, poking, or sealing. The proposed work seeks to develop a novel means by which force can be delivered and controlled at the tip of the serpentine arm. The focal advanced development and related application funded by TATRC lies in advancing the state of the art in minimally invasive surgery to the next level by using single ports or natural orifices when they are available. A number of other transition opportunities exist. For example, highly-articulated mechanisms such as these hold tremendous promise in support of robotic explosive ordnance disposal operations where by the mechanism could be used for exploration or disarming tasks.

B. Exploring Structural Phase Transformations Using Molecular Dynamics
Professor Kaushik Dayal, Carnegie Mellon University

The objective of this project is to advance the scientific understanding of structural transformations in metals and metallic alloys and develop new computational and theoretical techniques needed to achieve this goal. It is anticipated that this effort will provide a physical understanding of the atomic-level mechanism of structural transformations. In terms of computational and theoretical techniques, it will develop multiscale methods to deal with the fact that the critical processes occur on the scale of atoms and femtoseconds, while engineering interest is focused on the scale of meters and seconds. In this work, molecular dynamics, stability analysis, peridynamics, and multiscale approaches will be implemented to achieve the scientific objectives. The approach will involve a close collaboration between solid mechanics, mathematical analysis and computer calculations. The approach combines predictive ability of molecular dynamics with continuum (peridynamics) ability to compute at relevant length and time scales. If successful, this research will enable accurate predictions that can be used for materials design strategies, such as alloying and processing.

Structural phase transformations and twinning are keys to the behavior of a range of important advanced engineering materials: examples include high-strength transformation induced plasticity (TRIP) steels, superelastic alloys, ferroelectrics and nanotwinned metals. The findings on the physical mechanisms of deformation can in turn enable strategies for the design of new materials with optimized and targeted properties. For instance, superelastic alloys can absorb mechanical energy without significant permanent damage. In practical terms, this can enable structures that safely absorb kinetic energy (*e.g.*, blasts and impacts) and that can do this repeatedly from multiple hits at the same point. These properties are in contrast to most conventional ceramic systems that can be defeated by multiple hits at the same location. The research can enable functional and structural materials with enhanced reliability under repeated dynamic loading.

C. Level-Set Based Overset Grid Method for Vorticity Transport in an Incompressible Flow
Professor Jeffrey Marshall, University of Vermont

The objective of this project is to develop a new computational approach for simulating unsteady fluid flows around moving objects, such as rotor blades. The proposed computational approach applies the overset grid framework to the integral vorticity-velocity formulation for viscous fluid flows. The method employs a Cartesian "outer" grid surrounding the body for which numerous low-dissipation methods are available, and a body-fitted "inner" grid that surrounds the rotor blades and fuselage (see FIGURE 15). The inner grid serves to accurately resolve the boundary layer development on the body surface. The simulated flow is evolved on the coupled grids by solving the vorticity transport equation and the Biot-Savart integral. The chimera interpolation method was combined with a level-set distance function in which the zero level-set surface corresponds with the outer surface of the inner grid. The level-set function is used in computing the Biot-Savart integral for cells of the outer grid that overhang into the inner grid. This combination results in a highly efficient approach for partitioning cells of the outer (Cartesian) grid that overhang into the inner grid.

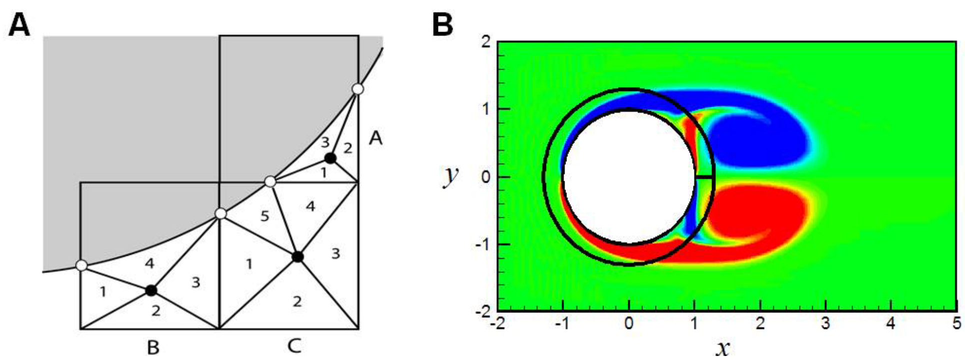


FIGURE 15

Proposed overset grid method. (A) The sketch illustrates three different types of overhanging grid cells: Type A with three sub-elements, Type B with four sub-elements, and Type C with five sub-elements. The region inside of the inner grid is shaded gray. Intersection points at which the level set function changes sign are indicated by open circles and the centroid point of each overhanging cell is indicated with a filled circle. (B) The figure illustrates the simulated vorticity field for impulsive flow past a circular cylinder.

The overset grid-level set integral vorticity transport method was tested for two and three-dimensional flows with both fixed and moving bodies. These tests uncovered a number of strengths and weaknesses in the method and a number of steps were taken to improve the numerical method to address the weaknesses. The validation tests conducted include: (i) uniform flow past a stationary circular cylinder, (ii) uniform flow past a vibrating circular cylinder, and (iii) uniform flow past an elliptical cylinder at a finite angle of attack with different ellipse aspect ratios. All validation tests conducted exhibit excellent comparison with available experimental data and prior computational results based on other methods.

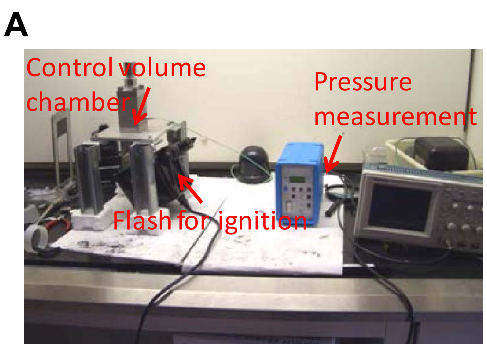
It is anticipated that this research will extend a previously-published method by Brown[1] for simulating rotorcraft-related flow fields by replacing the lifting-line approximation by a direct numerical solution for the vorticity shed from the body using an overset grid approach, where the outer grid is essentially the method used by Brown and the inner grid is an unstructured or body-fitted grid surrounding the body. If successful, the project will enable integral vorticity-velocity approaches to compete successfully with direct Navier-Stokes solutions for rotorcraft flow computations, allowing for more accurate solution of shed vorticity fields and interaction of shed vortices with downstream bodies.

D. Characterization of Ignition and Combustion of Nanowire-based Energetics

Professor Xiaolin Zheng, Stanford University

The objective of the effort is to develop new characterization methods that require only milligram level of nano-thermites and have the potential to predict their behavior at larger scale. Specifically the researcher will undertake an experimental study of ignition and combustion properties of nano-thermites on centimeter scales (or smaller). There are two major research challenges for the experimental efforts: to develop methods to ignite thermites for the small scale experiments with reliable performance, and to integrate high speed measurement systems to obtain sufficient data to extract the burning rate of thermites. Through these small scale experiments, the goal is to understand the dependence of ignition and burning speeds on the physical and chemical properties of nano-thermites and develop models to predict their behaviors on the larger scale.

To achieve these objectives, the researcher plans to develop a flash ignition method to initiate the reactions of nano-thermites and understand the ignition mechanism and processes. The investigator built a constant volume chamber and will use the apparatus to test the flash ignition method and measure the heat release rates of various nano-thermites (see FIGURE 16).



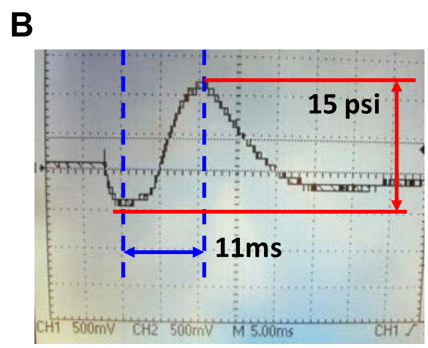


FIGURE 16

A constant volume chamber for testing the flash ignition method. (A) This is a photograph of the experimental setup of the control volume chamber to measure the heat release rate of thermites. It is equipped with a flash ignition unit outside the chamber and a pressure sensor to measure the heat release induced pressure rise. The data plot (B) is a preliminary pressure trace of flash ignition of 10mg of Al and CuO NPs. Further calibration of the pressure sensor is needed.

The investigator will also develop a new microchannel device with integrated Pt resistance sensors to measure the burning rates of nano-thermites and calibrate/validate the measurements with high speed camera. Finally, it is anticipated that Professor Zheng will synthesize metal oxide nanowires in order to provide the nanowire-based

[1] Brown. (2000). Rotor wake modeling for flight dynamic simulation of helicopters. AIAA Journal 38, 57-63.

thermites for the experiments that will focus on flame synthesis of metal oxide nanowires related to thermites, such as CuO, Fe_2O_3, WO_3 and MO_3 (see FIGURE 17).

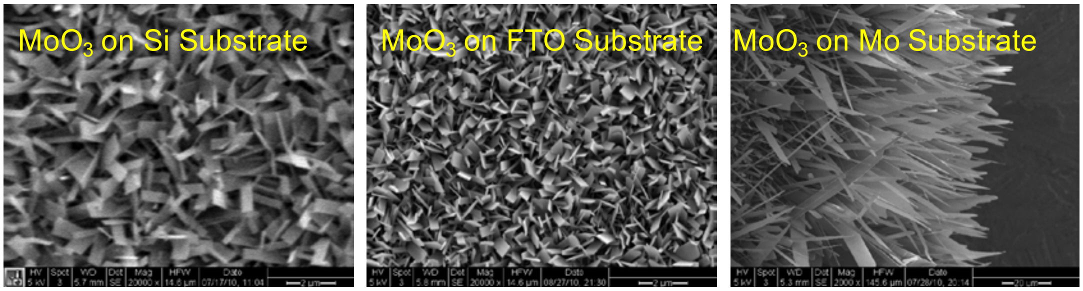


FIGURE 17

SEM images of flame synthesized one-dimensional MoO_3 nanostructures on Si, fluorinated transparent oxide and Mo substrates.

Energetic materials are critical to the propulsion performance in gun and missile systems of interest to the Army. First, the simple and economic flash method can be used to replace sparks and hotwires to initiate reactions of Al nanoparticles (NPs). Second, the Al NPs can be used as additives to gaseous, liquid and solid fuels to achieve homogeneous and volumetric ignition for combustors and engines. Finally, the proposed small scale experiments will provide valuable models to predict the large scale performance of nano-energetics.

VI. DIVISION STAFF

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Administrative Support Assistant

CHAPTER 11: NETWORK SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Network Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Network Sciences Division supports research to discover mathematical principles to describe, control, and to reason across the emergent properties of all types of networks (*e.g.*, organic, social, electronic) that abound all around us. The unprecedented growth of the internet, the tremendous increase in the knowledge of Systems Biology, and the availability of video from US military operations have all led to a deluge of data. The goal of the Network Sciences Division is to promote basic research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. In addition to advancing worldwide knowledge and understanding of networks, the research efforts managed in the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund research efforts, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates efforts with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division also coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Mechanical Sciences Division's Program Areas also interface with the Network Sciences Division to understand the interplay between learning and manipulation and locomotion in robotic systems. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Network Sciences Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, and (iv) Intelligent Networks. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The objective of this Program Area is to develop the theory and tools, through appropriate application and creation of relevant mathematics, to ultimately model, analyze, design, and control complex real-time physical and information-based systems, including distributed and embedded, networked autonomous and semi-autonomous, non-linear, smart structures, and decentralized systems. This Program Area invests in fundamental systems and control theory and relevant mathematical foundations for areas of control science such as multi-variable control, non-linear control, stochastic and probabilistic control distributed and embedded control, and multi-agent control theory. Further, the Program also involves innovative research on emerging areas such as control of complex systems and theories for the design of large heterogeneous multi-agent teams with desired emergent behaviors. This Program Area is divided into two research Thrusts: (i) Intelligent Control and (ii) Multi-agent Systems. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Intelligent Control Thrust involves research topics focusing on non-traditional approaches to control with focus on the Army's interest in basic research on intelligence, embedded in a single agent operating in highly uncertain, clustering, and complex environments. The Multi-agent Systems Thrust involves research focused on extending the mathematical foundations of distributed system theory, with a focus on basic research in the massive-scale, low cost, highly distributed agents cooperating over networks in highly uncertain, clustering, and complex environments. In addition, research focuses on the design of emergent behavior for heterogeneous multi-agent systems, accommodative-cooperative-collaborative theory of multi-agent behavior and interaction, and multi-player/multi-objective game theory.

2. Decision and Neuro Sciences. The goal of this Program Area is to develop theoretical foundations, models, and algorithms to support timely, robust, near-optimal decision making in highly complex, dynamic systems operating in uncertain, resource-constrained environments with incomplete information when facing a competent, thinking adversary. This Program Area is divided into two research Thrusts: (i) Numerical Optimization and Inference Modeling and (ii) Phenomenology: Cognitive and Neural Processes. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Numerical Optimization and Inference Modeling Thrust includes research efforts focusing on the development of a math-based framework for representing stochastic information flow, the design of algorithms (stochastic-based) for generating and selecting optimal plans of action, the development of models to adequately account for stochastic and highly heterogeneous information flow, and seeks to quantify sociological factors inherent in information. The Phenomenology: Cognitive and Neural Processes Thrust includes research efforts with the goal of identifying sociological implications, biases related to information content, and the integration and advancement of decision sciences results related to decision making, cognitive and neural behaviors. Based on operations-research methodologies such as modeling, simulation and numerical optimization, this Program Area includes a significant multi-disciplinary emphasis, specifically with neuroscience, to address the complex, multi-dimensional decision frameworks in today's asymmetric warfare.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research efforts to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from

heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research efforts to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

C. Research Investment

The total funds managed by the ARO Network Sciences Division for FY10 were $11.4 million. These funds were provided by multiple sources and applied to a variety of Program Areas, as described here.

The FY10 ARO core (BH57) program funding allotment for this Division was $4.2 million. The DoD Multi-disciplinary University Research Initiative (MURI), and Defense University Research Instrumentation Program (DURIP) provided $4.1 million to programs managed by the Network Sciences Division. In addition, congressional earmarks provided $2.3 million. Finally, $0.8 million in FY10 was provided through other sources for use in the Presidential Early Career Award for Scientists and Engineers (PECASE) program, the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) program, and a DARPA program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, “new starts”), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Paths Ahead in the Science of Information and Decision Systems (Boston, MA; 12-14 November 2009). The goal of this workshop was to bring together leading researchers from around the world in the fields of systems and control, networks and networked systems, estimation, inference and learning, and optimization and decision sciences, to discuss where the synergistic areas of future research are. The outcome was a report identifying potential key areas of research, which will be followed-up on by the program manager.

2. Third Annual North American School of Information Theory (Los Angeles, CA; 5-8 August 2010). The objective of this workshop was to bring top information theory researchers together to discuss new areas of information theory, including how the theory applies to wireless tactical networks and to familiarize information theory graduate students and post-docs with new research, including tactical networking. This workshop brought together experts in academia and the government as well as top graduate students to discuss emerging concepts in information theory.

3. Frontiers of Controls, Games, and Network Sciences (Austin, TX; 19-21 February 2010). This workshop focused on the impact of new analytical tools in the areas of controls, games, and network science on military wireless networks as well as commercial networks. This workshop brought together experts in academia, industry, and government laboratories to discuss new advances in applying control systems and game theory to wireless networking. This workshop facilitated cross-disciplinary interactions to help advance network science, particularly as it applies to wireless networking. This interaction will be likely to lead to cross-disciplinary collaborations that will ultimately lead to advances in wireless network science that can be applied to the tactical network as well as other areas of interest to the Army.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Network Sciences Division; therefore, all of the Division’s active MURIs are described in this section.

1. Determining the Mathematical Basis of Swarming. This MURI began in FY05 and was awarded to a team led by Professor Vijay Kumar at the University of Pennsylvania, with participation from researchers at the Massachusetts Institute of Technology (MIT), Yale University, and the University of California, Santa Barbara. The goal of this research is to understand the mathematical basis of swarming and its potential applications to cooperative control of tasks of all types, including the control of formations, the management of sensor networks, and the dynamics of achieving a consensus in a rapidly changing environment. This research effort will draw inspiration from biological paradigms and create a mathematical basis for modeling, analysis, and synthesis of swarming systems that are applicable to cooperative control tasks of all types, including the control of formations, the management of sensor networks, and the dynamics of achieving a consensus in a rapidly changing environment. The project consists of four research approaches: the modeling of group-behaviors in biology, the analysis of group behaviors, the synthesis of novel controllers for networked groups of vehicles, and experimental demonstrations and validation.

Future Army vehicle networks will perform a wide variety of coordinated sensing, motion and target prosecution. Coordination algorithms with the required scalability and correctness properties resulting from this project will enable future groups of robotic vehicles to be autonomous and adaptive in the face of communication constraints. The high levels of autonomy and robustness will allow future Army robotic teams or mixed human-robotic teams to carry out tasks with guaranteed performance. Specific applications are numerous. The tools from this project will enable new biologically-inspired control paradigms for swarms that will be usable in the context of adaptive tracking, surveillance, and navigation. The tools will also enable a solution to the problem of determining when an observed group exhibits normal behavior and when it exhibits atypical behavior - which has significant implications to homeland security and warfare. This technology will also enable monitoring and surveillance applications on geological and ecological scales previously prohibited by practical considerations and will provide tools for a host of security and surveillance applications.

2. Neuro-Inspired Adaptive Perception and Control. This MURI began in FY10 and was awarded to a team led by Professor Panagiotis Tsiotras of the Georgia Institute of Technology, with participation from researchers at the Massachusetts Institute of Technology and the University of Southern California. The objective of this MURI is to investigate a new paradigm based on "perception/sensing-for-control" to achieve a quantum leap in the agility and speed maneuverability of vehicles. The team will leverage attention-focused, adaptive perception algorithms that operate on actionable data in a timely manner; use attention as a mediator to develop attention-driven action strategies (including learning where to look from expert drivers); analyze the saliency characteristics of a scene to locate the important "hot-spots" that will serve as anchors for events; make use of fused exteroceptive and proprioceptive sensing to deduce the terrain properties and friction characteristics to be used in conjunction with predictive/proactive control strategies; and will study and mimic the visual search patterns and specialized driving techniques of expert human drivers in order to develop perception and control algorithms that will remedy the computational bottleneck that plagues the current state of the art.

This MURI will have significant benefits for the Army in the field and off the field, such as increasing vehicle speed and agility in direct battlefield engagements, as it will increase the chances of evading detection by the enemy or of escaping an ambush. As confirmed by several Army studies, the difficulty of successfully engaging and hitting a target increases disproportionately with the target speed. Support logistics will also become safer and more effective as even moderate increases in speed can largely increase the capacity of convoys and the throughput of the supply lines of materiel. Finally, the results of this research will contribute to the development of realistic off-road high-speed simulators for training special forces and other military and government personnel.

3. A Unified Approach to Abductive Inference. This MURI began in FY08 and was awarded to a team led by Professor Pedro Domingos at the University of Washington. The goal of this research is to investigate Markov Logic Networks as a model to study human cognition, specifically the process of human analysis of seemingly disparate, voluminous data to explain the most possible cause for a set of observations.

Abduction is the process of generating the best possible explanation for a set of observations. While this calls for generation of a logical argument, observed data invariably contain inconsistencies. The research team has been investigating the use of Markov Logic Networks, a formalism that combines first order predicate logical and statistical reasoning to combine logical rigor with soft constraints, to capture domain knowledge. The task of generating explanation can then be looked upon as the inverse of forward chaining with the greatest

probability/weight. To make such an automatic system scalable/practical this research effort involves (i) cognitive science based heuristics for guiding generation of most likely proof trees, (ii) integration of low level sensor data with potential imprecision into the reasoning process, and (iii) parallel and distributed schemes for speeding belief propagation and proof construction, etc. Finally, the MURI team is working on several case studies to validate their approach; this includes generation of explanation for how a Capture the Flag game is played, based on GPS traces. The ability to fuse information of different kind, and to reason about it at higher cognitive level, is relevant to improving situational awareness for Soldiers and commanders in a battlefield.

4. Cross-Disciplinary Approach to Modeling and Analysis of Wireless Networks. This MURI began in FY05 and was awarded to a team led by Professor J.J. Garcia-Luna-Aceves at the University of California - Santa Cruz. The goal of this research is to expand the knowledge of theory of networks as it applies to wireless ad-hoc networking.

The new theories developed during this research will be used to develop a better understanding of ad-hoc network performance and to improve networking protocols. In addition, insights from wireless communications networks derived from this program will contribute a new area of network science. This MURI has already generated several noteworthy accomplishments, including results in routing, network capacity, mobility models, and disruption tolerant networking. There have also been contributions in network coding, both theoretical and for issues with applying network coding to mobile *ad hoc* networks.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY10.

E. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY10.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Conservation of Information Principle for Intelligent Systems. This new HBCU project is led by Professor William Lawless of Paine College. The goal of this project is to develop mathematical models of dynamic behavior in social groups and organizations. In particular, the PI will investigate whether traditional techniques, such as Fourier Transforms and differential equations, can be used to analyze the dynamics of social groups. The difficulty, however, is that data collected to validate proposed mathematical laws could have perturbations that make it useless for validating the proposed laws. The focus of the research will be to cleanse the data of illusions and other effects before using them to validate mathematical laws for dynamics of social organizations. The proposed effort is relevant to the Army’s recent interest in net-centric warfare as a strategy.

2. Formalization of Human Behavior in Human-Machine Interactions. This new HBCU project is led by Professor Celestine Ntuen of the North Carolina Agricultural and Technical University. The goal of this research effort is to study the impact of humans in the loop on analysis of system-of-systems. Human beings are too complex to be easily reducible to a few parameters and consequently, the proposed work will evaluate the minimum set of human traits necessary to model prediction, anticipation, reasoning, and the learning aspects of human intelligence. The results from this effort are likely to be applicable for the development of tools for use in analyzing realistic battlefield situations through simulation.

3. Analysis of Multiresolution Coding for Orthogonal Frequency Division Multiplexing. This new HBCU project is led by Professor Dhadesugour Vaman at Prairie View Agricultural and Mechanical University. The goal of this research is to investigate algorithms for the transport of data to support multimedia applications in mobile *ad hoc* networks (MANETs) and sensor networks. Investigations will be performed with the goal of

increasing efficiency, enhancing security, and facilitating cognitive radio functionality. The effort is divided into four tasks. The first task will combine unequal bit error protection of non-symmetric higher order modulation with multiresolution video coding techniques, which divide the video into basic and enhanced data. The second task will develop an anonymity index in order to evaluate how various network and routing protocols affect the anonymity of a node. In the third task, joint medium access control/physical layer joint design will be investigated in the context of bandwidth and energy efficiency for cognitive radio. The use of orthogonal frequency division multiple access is suggested, since it offers maximum flexibility in bandwidth usage, but this results difficult non-convex optimization problem, which will be investigated. In the last task, a compressive sensing technique will be investigated, where successive reconstruction at the decoder side is used to avoid predetermined key package in transmission. The results from these tasks will be demonstrated on an existing MANET test bed. Given that multimedia traffic is an increasing is of ever increasing importance to tactical communications, this research will be applicable to future tactical networking protocol design.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Network Sciences Division managed three new DURIP projects, totaling $0.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of autonomous vehicle control in uncertain environments and strategies for building wireless networks in an ad-hoc and dynamic fashion.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Network Sciences Division.

A. Reliability-based Design Optimization (RBDO) under Input and Model Uncertainties

Professor K. Choi, University of Iowa, Single Investigator Award

Reliability-based design optimization (RBDO) has been applied to various engineering applications such as stamping, vehicle design with durability, and noise, vibration, harshness (NVH) analysis, where accurate sensitivities of performance functions are available. However, many engineering applications lack models of accurate sensitivities of performance functions. These include systems such as drive train, crashworthiness, micro- or nano-mechanics, and fluid-structure interactions. This research focuses on developing a sequential sampling-based dynamic Kriging (SS-DKG) method that can generate a highly accurate surrogate model in an efficient manner compared to existing surrogate modeling methods, and therefore lead to more effective designs. Designing vehicle or other complex systems involves identifying effects from numerous interacting factors. Oftentimes these effects are best simulated using physics-based models, which are highly detailed and computationally challenging. When detailed physics-based models are not practical or available, finding effective surrogate models is important. Traditional Kriging methods do not maximally use the information from the evaluated samples due to the fixed form of the mean structure (*i.e.*, basis functions). That is, even if higher-order terms are used, fixed-order basis functions may not be the best selection to describe the pattern of nonlinearity of the mean structure.

Professor Choi and colleagues recently developed a sampling-based approach that is more accurate than the traditional Latin hypercube methods. The reason for this is that the accuracy of the surrogate model may not be enhanced by simply using higher-order terms. Therefore, the problem is how to find the optimal set of basis functions such that the surrogate model will have the highest accuracy. To handle this question, an optimization problem is proposed that dynamically solves for the minimum cost (error) in selecting sampling testing points. This sequential sampling technique uses the bandwidth of the prediction interval obtained from the Kriging method and is integrated with the DKG method to find the region where the surrogate model has the least prediction confidence, which means that the region is highly nonlinear. Once accurate surrogate models are constructed, then RBDO can be carried out for problems for which sensitivities are unavailable. The mathematical formulation of a general RBDO problem is expressed as an optimization problem minimizing cost where the cost can be measured by variables related to physical parameters of the possible designs. Using accurate surrogate models and using a Monte Carlo simulation (MCS), the probabilistic constraint in the RBDO formulation can then be evaluated. This RBDO procedure is called the sampling-based RBDO since it uses MCS to calculate the probability of failure and its sensitivity. Computational models of this sampling based approach have been developed and simulations and optimal solutions have been derived for specific materiel components. These numerical methods have been shown to be highly scalable and amenable for parallel processing. Further, mathematical examples show that the proposed sampling-based approach yields a very accurate optimum design compared to existing methods. An important next step is testing designs generated by the RBDO method by manufacturing actual designed components and then testing strength, weight, reliability and other properties. The newly developed SS-DKG Matlab toolbox has been integrated into University of Iowa's numerical software platform and is compatible with software at the Army Tank and Automotive Research, Development and Engineering Center (TARDEC). The Iowa RBDO platform is installed on the TARDEC High Performance Computing system and is being used to design frame components of Army vehicles.

B. Methodology for Programming under Probability Constraints

Professor M. Lejeune, George Washington University, Young Investigator Program Award

Optimization tools are required to address uncertainty, which is usually part of any decision process. Given that an optimization problem involves an objective function as well as constraints, addressing constraints having probabilistic bounds is an important problem to solve effectively and efficiently. This research addresses

developing improved algorithms to solve problems involving uncertainty by integrating and expanding knowledge from the pattern recognition into the stochastic programming discipline. This new methodology involves: (i) the development of a modeling framework of stochastic constraints via combinatorial patterns, (ii) the design of exact algorithmic techniques to generate combinatorial patterns, and (iii) the derivation and solution of a deterministic equivalent or tight approximation of the original stochastic problem.

The uniqueness of the approach stems from the investigation of the synergistic interactions between stochastic programming and pattern recognition fields. The motivation for developing a pattern-based framework for stochastic optimization problems is the following. The performance of complex systems typically depends on a set of adopted decisions and the values taken by multiple stochastic, uncontrollable random variables. Combinatorial patterns have the capability not only to identify the variables that can individually influence the system but also to capture the collective effect of the values of these variables on the system. The use of combinatorial patterns will enable solving stochastic problems in which the uncertainty is very finely represented (*i.e.*, represented by an extremely large number of scenarios). This is a key distinct feature and outcome compared to currently available solution methods.

The modeling framework introduces the concept of a p-sufficient realization, where a p-sufficient realization is a vector having cumulative probability that is at least equal to the prescribed reliability level p. This implies that if all the requirements defined by the p-sufficient realization are satisfied, then the probabilistic constraint holds. A binarization process is carried out using a consistent set of cut points. The consistency property of a set of cut points preserves the disjointedness between the set of p-sufficient and p-insufficient realizations. This means that each p-sufficient realization will have a binary image that differs from the binary images associated with any of the p-insufficient realizations. An advantage of the binarization process is that it allows the elimination of a large number of realizations (scenarios) based on easily detectable reasons. The combinatorial p-patterns provide a compact representation of conditions that are sufficient/minimal for the satisfaction of a stochastic constraint. The next task is to derive those patterns, possibly the ones deriving the minimal/least demanding conditions for the satisfaction of the probabilistic constraint. It is shown that p-patterns have a large degree at least equal to the dimension of the random vector. Two linear programming formulations and two mixed-integer programming formulations are proposed for the generation of p-patterns. The constraints and decision variables of the mathematical programming formulations are defined in such a way that any feasible solution defines a "promising" p-pattern. A promising p-pattern involves cases where the pattern defines conditions that are equal or close to the minimal requirements that need to be attained for the satisfaction of the probabilistic constraint. The p-patterns allow the formulation of a linear programming problem that is an inner approximation of the original stochastic problem and that can be solved with any linear programming solver. Also, the team derived an approach for the concurrent generation of a p-pattern and the solution of the deterministic equivalent of the stochastic problem. The optimal solution of this problem defines the p-pattern that imposes the minimal requirements for the stochastic constraint to hold. A mixed-integer programming problem is formulated that contains one binary variable for each cut point used for the binarization of the probability distribution. The number of cut points is typically much, much smaller than the number of scenarios. Thus, the number of binary variables (and thus, most likely, the solution time) is not an increasing function of the number of scenarios used to describe random variables. This result explains why this method is very successful in solving stochastic programming problems in which the uncertainty is very finely characterized. This work has generated preliminary results showing that complex stochastic problems, in which up to 50,000 scenarios represent the random, can be consistently solved to optimality within a few seconds. These results and future work on this project in the next two years will provide capabilities for Army commanders to make more optimal decisions under uncertain conditions, which will be important for complex operational activities.

C. Theory of Geometric Observers and Particle Filtering in Controlled Active Vision

Professor Allen Tannenbaum, Georgia Institute of Technology, Single Investigator Award

This research explores the theory and practice of visual information in a feedback loop, the underlying problem of controlled active vision. Controlled active vision requires the integration of techniques from control theory, signal processing, and computer vision. Visual tracking provides an important example of the need for controlled active vision. Tracking in the presence of a disturbance is a classical control issue but because of the highly uncertain nature of the disturbance, this type of problem is very difficult. Visual tracking differs from

standard tracking because the feedback signal is measured using imaging sensors. In particular, it has to be extracted via computer vision and image processing algorithms and interpreted by a reasoning algorithm before being used in the control loop.

In FY10, the investigators explored 3D tracking either from range or stereographic data, using methods that are a combination of particle filtering as well as active contours. The researchers then employed particle filtering and active contours to estimate the global motion of an object and its local deformations, respectively. The team used this data to develop a novel information-theoretic approach to segmentation that uses the all the statistical data in the tracking sequence. The key idea underpinning this segmentation approach is that for a properly selected subset of image features, the "overlap"' between the informational contents of the object and of the background has to be minimal. In other words, if one thinks of the active contour as a discriminator that separates the image pixels into two subsets, then the optimal contour should minimize the mutual information between these subsets. Note that for the case at hand, minimizing the mutual information is equivalent to maximizing the Kullback-Leibler divergence between the probability density functions (PDFs) associated with the "inside" and "outside"' subsets of pixels. However because of computational efficiency instead of the divergence, the investigator proposed to maximize the Bhattacharyya distance between the PDFs. A region-based active contour model driven by the Bhattacharyya gradient flow was adopted for its robustness to noise in a cluttered environment. The proposed algorithms take advantage of both range information and contour-tracking while at the same time dealing with the challenging situation that occurs when objects being tracked disappear from the image domain and reappear later. To cope with this problem, a PCA-based shape analysis was proposed, which defines a shape similarity energy to find target candidates that are as close as possible to the template shape obtained online using the previous segmentations, rather than the prior training shapes. Experimental results show the robustness and practicality of the proposed algorithm for real tracking problems.

Furthermore, the researcher has developed a non-rigid approach to jointly solve the tasks of 2D-3D pose estimation and 2D image segmentation. In general, most frameworks that couple both pose estimation and segmentation assume that one has the exact knowledge of the 3D object. However in non-ideal conditions, this assumption may be violated if only a general class to which a given shape belongs to is given (*e.g.*, cars, boats, or planes). Thus, the key contribution in this work is to solve the 2D-3D pose estimation and 2D image segmentation for a general class of objects or deformations for which one may not be able to associate a skeleton model. Moreover, the resulting scheme can be viewed as an extension of a previous framework in which the research team included the knowledge of multiple 3D models rather than assuming the exact knowledge of a single 3D shape prior. These recent accomplishments are relevant to building autonomous ground vehicles and robots that are likely to be an integral part of future combat forces.

D. Analysis and Optimization of Cognitive Radio

Professor Mike Pursley, Clemson University, Single Investigator Award

Cognitive radios adapt to the current communication channel conditions to improve network performance. If cognitive radios are provided with the right protocols, they have the potential for more than an order of magnitude improvement in throughput compared to conventional tactical radios. The objective of this research is to investigate the use of different protocols in different channel conditions in the context of cognitive radio, including effects of fast fading and other high rate variations of the channel.

In FY10, low-complexity adaptive protocols were developed that are appropriate for tactical packet radio networks. Throughput performance that is near the information-theoretic limit has been demonstrated for protocols that do not require channel measurements and need no pilot symbols or other overhead. The feedback required by the protocols is only a few bits in each acknowledgment packet and the protocols can tolerate a reasonable amount of delay in the limited feedback that they use. The resource consumption metric that has been devised has been shown to give a basis for cooperation among the radios in a network. This may be the first quantitative measure of communications resources that is suitable for use in adaptive protocols for tactical cognitive radio networks. In addition code-modulation libraries for tactical cognitive radio were developed. The same demodulator statistics that were used for adaptive protocols are employed to improve soft-decision decoding. Protocols have been devised and evaluated for initial power adjustments, adaptation to time varying propagation conditions, and combined channel access and adaptive spreading in tactical direct-sequence spread-spectrum dynamic spectrum access networks. Adaptive frequency-hop transmission protocols have also been

investigated to combat time-varying propagation conditions and interference. The design and evaluation of cross-layer protocols that use receiver statistics or other physical-layer information typically require embedded simulations of each radio's demodulator and decoder. The embedded simulations of the decoder are especially computationally intensive in tactical radios that employ iterative decoding to combat noise and interference.

E. Cognitive Opportunistic Communications and Cognitive Cross-layer Protocol Stack Design

Professor Ramesh Rao, University of California, San Diego, Single Investigator Award

Cognitive networking will expand the concept of cognitive radio to have not only the physical layer adapt to the environment, but also to the network and transport layers. The goal of this research effort is to investigate the cognitive mechanisms that will control this adaptation in the context of mobile *ad-hoc* networks. The investigator has been studying cognitive select protocols for a new environment based on previous observations of similar channels. In this research, Bayesian Networks (BNs) are used to create a representation of the dependency relationships between significant parameters spanning transport and medium access control (MAC) layers in single hop and multi-hop wireless network environments. In single hop networks, graphical models were created from historical data observed from the protocol stack and verified their usefulness. Then the developed BN models were used to mitigate one of the problems of the TCP protocol, which does not have any mechanism to infer when congestion occurs in the network and therefore waits untill some packets are lost for reacting to congestion in the network. Such a reactive nature of TCP leads to a waste of precious network resources, like bandwidth and power.

With the help of BN structure derived from network environment and current network state, an algorithm was designed in FY10 to infer in advance the congestion state of the network. BNs have been constructed for different network environments by sampling network parameters on-the-fly in simulated network environments. The congestion state of network can be predicted, using BNs, with quite good accuracy given sufficient training samples and the current value of the TCP congestion window.

The investigator revealed several results from this research, including that: (i) BN is a useful tool for cognitive networking to determine, represent and exploit the probabilistic dependencies and conditional independencies between protocol parameters, (ii) by exploiting BN, an inference engine can be design to accurately predict the behavior of protocol parameters, and (iii) the influence of the data size used for training on the accuracy of network parameter behavior prediction can be determined using these techniques. This research will lead to tactical cognitive radio networks that will have better data throughput by adapting the environment and reduce the work load in both pre-configuring radios and changing the configuration in the field to adapt.

F. Neuroscience-enabled Complex Visual Scene Understanding

Professor Laurent Itti, University of Southern California, Single Investigator Award

Professor Itti has been working on formalizing an autonomous system for vision based on hierarchical Bayesian Inference system that was inspired by recent results in cognitive science on human vision system. Hypotheses based on objects in a visual scene are generated "bottom up" from sensor data. These hypotheses are then refined and validated "top down" when complex objects, hypothesized at higher levels, impose new feature and location priors on the component parts of these objects at lower levels.

To efficiently implement the framework, the PI systematically utilized the concept of bottom-up saliency maps to narrow down the space of hypotheses. In addition, the PI let the system hallucinate top-down maps (manufacture its own data) at low levels given high-level hypotheses to overcome missing data, ambiguities and noise. The implemented system has been tested against images of real scenes containing simple 2D objects against various backgrounds. The system correctly recognizes the objects in 98.71% of 621 video frames, compared to SIFT (a system based on the notion of scale-invariant key features of an object for identification), which achieves 38.00%.

The current framework was expanded with a few new modules for bottom-up processing. The module V2 (for instance) now implements the tensor voting framework proposed by G. Medioni. This boosts the edges and makes them more salient if they are continuous. The Contours module implements a simple edge tracking algorithm that prefers edges with the same orientation, magnitude and distance. The contours are then

approximated with lines. Lastly the 2.5D Sketch module provides 2D shape recognition with similarity transformation. This is done with a Generalized Hough transform to propose shapes. The shapes are then evaluated using a directional chamfer matching for efficiency.

The investigator and colleagues have explored a method for tuning the various parameters in the system using the notion of bottom-up and top-down processes (see FIGURE 1). This can be seen as biasing various detectors to give different results. One classic example is choosing a threshold for edge detectors. The system was developed to explore the parameter space using the current framework. This was done by setting the initial threshold value to a high number, which reduced the amount of data to the system. For example, setting the edge threshold in (module) V1 resulted in fewer edges available to (module) V2. The system will then propose a shape, evaluate a probability for it, and send a bias signal to reduce the threshold values in regions where there are no edges. This results in two outcomes. Either the shape is found, in which case the probability will increase due to the additional correct edges, or the shape is not found, which will reduce or keep the probability the same (investigators determined that a shape is found if more the 75% of the edges contribute to the match). The process will then continue as long as the probability is increasing or stop if it is not. Even though this is an iterative process, only about three iterations on average were required to extract the shape. The use of saliency maps for bottom-up processing and voting/Markov decision process approximate the human visual system. The proposed system could be part of future US Army robotic systems that need to deal with the highly dynamic situations and may have use where control and perception need to work hand in glove.

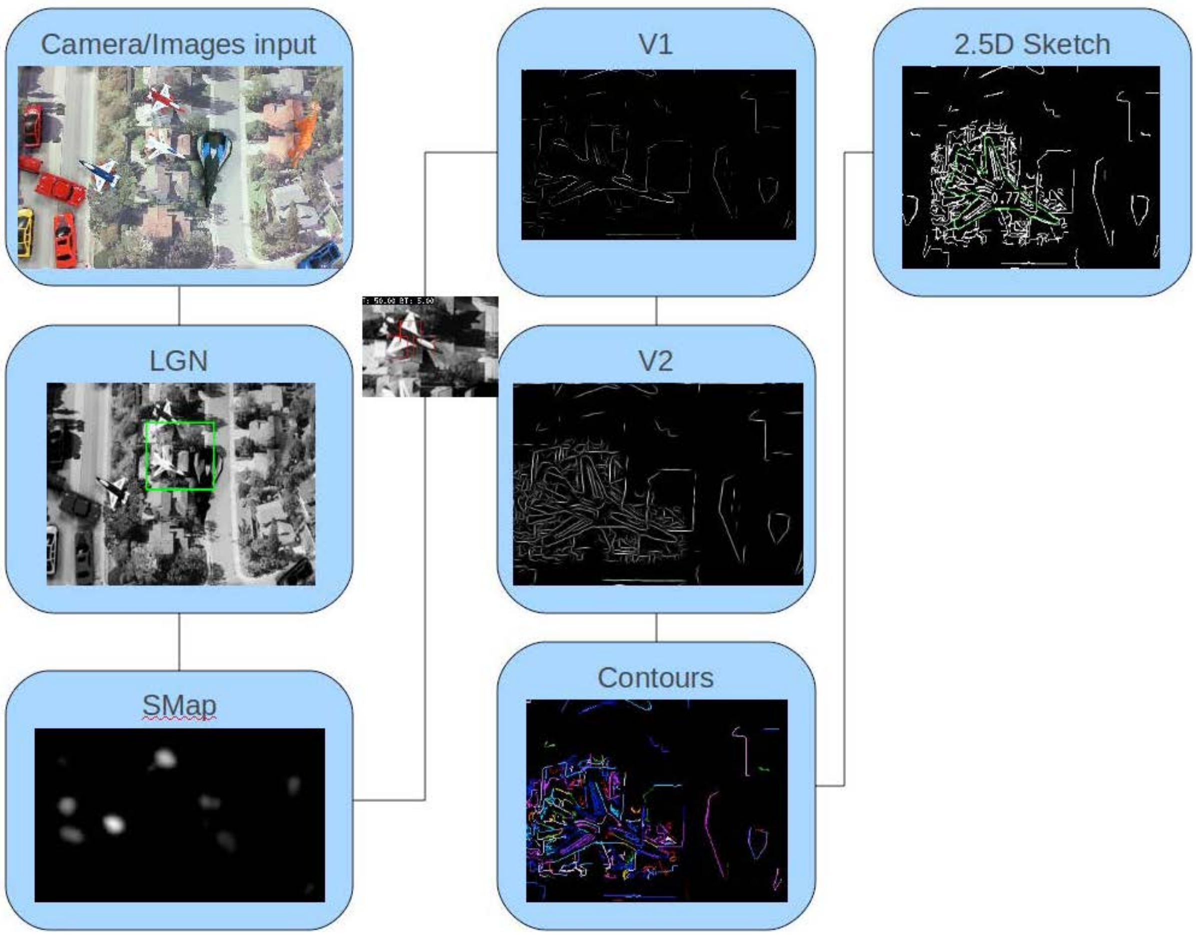

FIGURE 1

Stages of new architecture and algorithm in bottom-up processing of frames for object recognition. The advancements in FY10 include modules V2 and 2.5D. Module V2 implements the tensor voting framework proposed by G. Medioni and boosts the edges making them more salient if continuous. The Contours module implements a simple edge tracking algorithm that prefers edges with the same orientation, magnitude and distance. The contours are then approximated with lines. The 2.5D Sketch module provides 2D shape recognition with similarity transformation.

G. Game Theoretic Models of Conflict and Social Interaction
Professor Asuman Ozdaglar, MIT, Single Investigator Award

The goal of this project is to bring techniques from Mathematical Game Theory to study social conflicts and interactions. The formalization of social interactions in a network setting provides the foundation for this research effort. More specifically, this research will study how beliefs are formed and information is spread in a society along with exploring game theoretic techniques and influences to the behavior of large groups.

The interactions between members of a group or society can be captured as a graph with the individuals formalized as nodes and the strength of the interactions captured by appropriate metric on the edges of a complete graph. Propagation of belief at each time step can then be characterized as a probability distribution over a pair of nodes exchanging messages, with either some consensus being reached between them or one of them forcing the other to his/her view. With this setting the temporal nature of the belief propagation can be characterized as stationary properties of the resulting Markov chains.

The PI and his research team recently demonstrated: (i) that beliefs across a network stabilize some stochastic, convex combination of the original beliefs, and (ii) that the network structure does play a role in whether beliefs of an intransigent member (*i.e.*, someone who does not change his/her opinion and who has vested interest in propagating misinformation in the society) propagate through the network. In particular the result revealed that if misinformation is fed from members on the bridge between two large connected components, then it will be accepted. The results of this project are advancing the study of human networks. It is expected that such results will play a major role in the decision making in the Army as it moves to asymmetric warfare within urban areas.

H. Biologically-Inspired Modeling and Learning of Gaits for Snake Robots
Professor Howie Choset, Carnegie Mellon University, Single Investigator Award

Snake robots are highly articulated mechanisms that can use their many degrees of freedom to thread through tightly packed volumes, transmitting data and retrieving samples from remote locations inaccessible to conventional machinery and people. These many degrees of freedom also offer a broad class of locomotion capabilities, which makes sense when their biological counterparts, snakes (which can crawl, climb, swim, etc.) are studied. The objective of this project is to develop new mathematics to describe the optimal locomotion of robots (*i.e.*, minimize energy) across the ground.

The investigators have successfully completed extensive video studies of snake motion to understand the key parameters in gaits of snakes and have put forth a learning algorithm based on gradient-search, to animate a snake robot across a flat surface. The researchers found that a significant characteristic of the learning algorithm is the sufficiency of relatively small samples to achieve over 70% accuracy in motion over flat surfaces. Future work will address motion across inclined surfaces. It is expected that in the future robots, and autonomous systems, will provide enhanced situational awareness for Soldiers in a battlefield, especially in urban settings.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Modeling and Performance Analysis for JTRS/SDR Waveform Evaluation

Investigators: M. Pursley and D. Noneaker, Clemson University, Single Investigator and DEPSCoR Awards
Recipient: Space and Naval Warfare Systems Command, Charleston (SPAWARSYSCEN)

The objective of this research is to devise adaptive transmission protocols that make optimal responses to deviations in channel quality to ensure reliable communications without causing excessive interference to friendly forces or civilians in the host country. These protocols are intended for use in future military cognitive radios and software radios. A related, but previously completed project by Professor Noneaker (DEPSCoR award) resulted in novel iterative, equalization-and-decoding algorithms for use in multipath fading channels. A set of channel models representing a broad range of tactical communication environments was developed for use in evaluation of the algorithms.

These results transitioned to SPAWARSYSCEN in Charleston, SC, and Professors Pursley and Noneaker participated in a study of JTRS waveforms for the recipient company. The researchers conducted a short-term study to evaluate techniques and protocols for using SDR waveforms in support of dynamic utilization of radio spectrum for increased range, capacity, and reliability of tactical radio networks. The PIs also assisted in identifying and developing models of time-varying wireless communication channels that allow a more comprehensive evaluation of the JTRS Wideband Networking Waveform (WNW) in the SPARWAR test bed. Professor Noneakers's channels models transitioned to test bed evaluations of the performance of the WNW and the Soldier Radio Waveform (SRW) on JTRS Ground Mobile Radio EDM hardware, and SPAWAR supplied them to ITT by for use in evaluations of the SRW. The results on protocols for dynamic spectrum utilization, developed under Professor Pursley's ARO grant, provide concepts that can be exploited for longer-term investigations at SPAWARSYSCEN for future cognitive radios and nearer-term software radios.

The improved channel models will benefit the JTRS and other SDR evaluations. The concepts developed during the research on adaptive protocols will benefit longer-term investigations of cognitive radio networks, dynamic spectrum utilization, and are relevant to applications of SDRs to tactical communications.

B. Advanced Radar Data Fusion: Multiple Input Multiple Output Sensor Acquisition System

Investigator: Rick Blum, Lehigh University, Single Investigator Award
Recipient: Missile Defense Agency (MDA)

The goal of this research is to discover new methods for energy-efficient signal detection and estimation for networks of dispersed sensors. Professor Blum has recently derived new theoretical results in energy efficient statistical signal processing with dispersed sensor networks. The investigator has developed a distributed sensor radar system that has transitioned to MDA where it is currently being tested with the MDA Multiple Input Multiple Output Sensor Acquisition (MIMOSA) System project. Professor Blum has also developed a method to reduce the number of transmissions in distributed sensor systems, which is directly applicable to the MIMO radar systems that the MIMOSA project is evaluating. Thus this ARO-sponsored discovery is also being tested under the MDA program for reducing transmissions for implementation in the next generation MDA systems. Preliminary results estimate the energy savings due to these new algorithms to be very large and therefore it is likely that the MDA will integrate them into new their new MIMO RADAR systems.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. High Throughput via Cross-Layer Interference Alignment

Professor Robert Heath, University of Texas, Austin

Interference alignment is a new concept that is receiving significant attention in the research community. It is a cooperative transmission technique designed to manage the interference in a large-scale network, such as a tactical MANET. Professor Robert Heath is currently investigating using multi-antenna MIMO techniques to implement interference alignment. This research will build upon some preliminary results of the PI in which he demonstrated the feasibility of interference alignment.

It is anticipated that this research will lead to the development of the mathematics necessary to understand the effects of overhead and synchronization on MIMO interference alignment techniques. In addition the results of this research will advance efforts to determine the feasibility of interference alignment.

B. Geo-spatial Abduction

Professor Venkatramana Subrahmanian, University of Maryland

Abduction is the process of explaining a cause from a set of observations. Geo-Spatial abduction is used to reason about the geographical cause or location related to observations of a given phenomenon, such as identifying the source of an outbreak when a disease is identified. This concept is widely applicable to both civilian (crime detection) and military (locations of weapons cache) situations. This approach must take into account the actions of an adversary who is likely to lead astray any efforts to discover his/hear actions.

The objective of this research effort is to determine a mathematical framework and associated algorithm that will allow formalization of socio-cultural factors of a geographical area and the actions of an intelligent adversary who seeks to cover his/her tracks, in the context of geo-spatial abduction. Specifically Professor Subrahmanian is attempting to identify a partner location with a given set of distance constraints regarding how far and how near the partner location can be to a corresponding observation, given that certain locations can, or cannot, be the site of the cause (due to geographical or cultural factors). The PI has proposed heuristics based on the set-covering problem and he has applied his approximate algorithm to determining the potential locations of weapons caches and has validated his algorithm against data on IEDs.

It is anticipated that the investigator will bring game theoretic techniques (*i.e.*, recast the problem to maximize the likelihood of a location being chosen by an adversary who, of course, would chose the least likely place to be detected) to counter adversaries that might hide their weapons cache sites. This approach is of relevance to current asymmetric wars in which U.S. forces are engaged, and in which forces are likely to be faced with in the future.

C. Strategic State Estimation in Uncertain and Mixed Multiagent Environments

Professor Prashant Doshi, University of Georgia

Human judgment of uncertainty suffers from various cognitive biases. In the military context, operators of autonomous vehicles such as unmanned aerial vehicles (UAVs) generally assess probabilities at levels that are not objectively justified. Some of the psychological issues that affect probability judgment include inaccuracy in verbally reporting probabilities and a lack of honesty in expressing the true probability assessments. The objective of this project is to take critical steps toward establishing a field-valid probability assessment and update techniques using a realistically simulated UAV setting. Furthermore the investigator will study and computationally model validated static probability assessments and probability updates.

The investigator will study the presence of cognitive biases in judgment and techniques. It is anticipated that the researchers will obtain valid probability assessments of cognitive biases using three large psychological studies in the context of the Georgia Testbed for Autonomous Control of Vehicles (GaTAC). GaTAC is a computer simulation framework for evaluating autonomous control of aerial robotic vehicles, such as UAVs (see FIGURE 2). It provides a low-cost and open-source laboratory alternative to highly complex and expensive simulation infrastructures. GaTAC deploys multiple instances of open-source flight simulators utilizing hyper-realistic 3D terrain data on a networked cluster of computing platforms. GaTAC provides a flight dynamics software module that translates high-level navigational actions to commands for the flight control surfaces. GaTAC will allow for maximum ecological validity of the studies in a laboratory setting. In contrast previous investigations of biases in judgment utilized simple settings in which the relevant probabilities were few, were given, and the calculations were often simple.

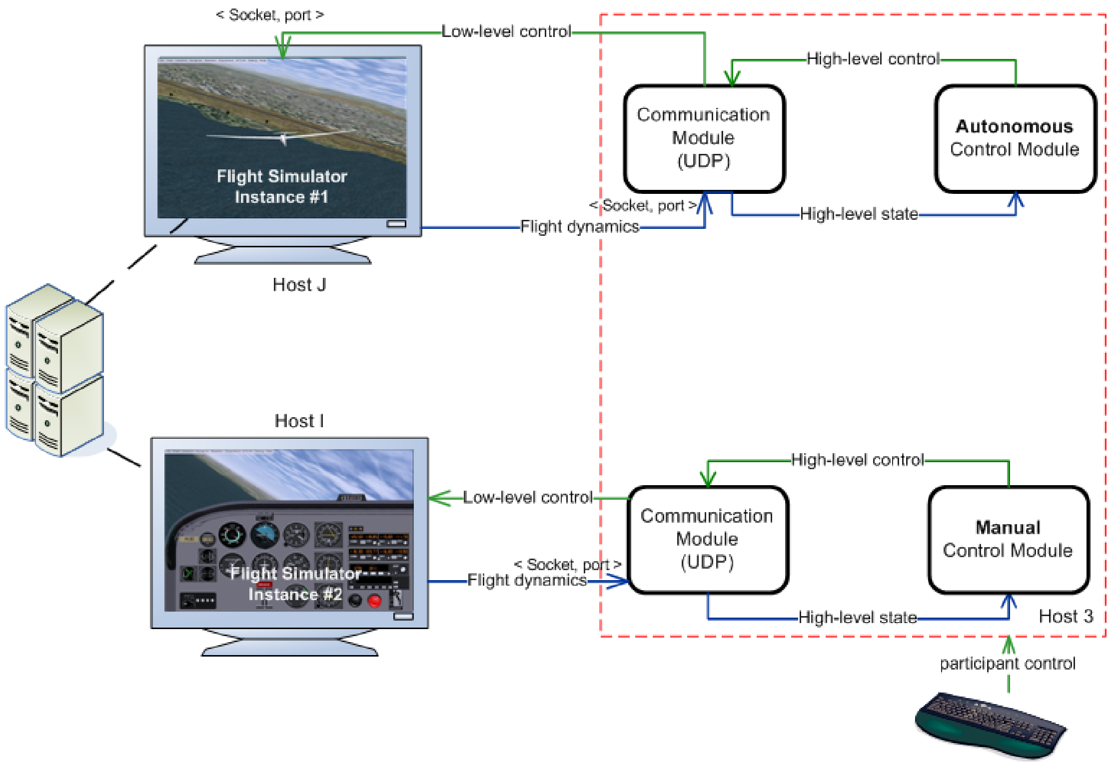

FIGURE 2

GaTAC Architecture. GaTAC is a computer simulation framework that is used to evaluate the autonomous control of aerial robotic vehicles.

The first component of the research effort is in progress, with a goal of investigating whether participants' verbal probability assessments are unreliable while seeking ways to validate the assessments. The primary alternative to direct verbal expressions is to determine preferences between betting on the outcome of the predictive probability event and on events with clear, objectively specified probabilities. This study will investigate whether the verbal reports are consistent with degrees of uncertainty as inferred from the choice data.

Previous findings indicate that humans tend to be generally overconfident; they assess probabilities of their predictions higher than objectively justified and at high levels of confidence. While candidate models of probability assessment exist, they suffer from two limitations: (i) there is no consensus on these models among the research community, and (ii) these models result from domain-general approaches in simple settings that do not guarantee the validity of the findings in complex military tasks. Uncertainty in realistic settings is often difficult to judge and is not objectively specified to the decision maker.

The use of simulated UAV settings allows for maximum field-valid assessments in a laboratory setting. This study will lead to future investigations of the cognitive biases of not only an operator of vehicles but also of an opponent participating in a strategic game. The outcomes of this research will ultimately lead to techniques that

facilitate valid and honest assessments of uncertainty and updates of the probabilities. Important military decisions are often predicated on the probabilities of predictive events reported by the operator.

D. Probabilistic Tracking and Trajectory Planning
Professor Mark Campbell, Cornell University

Current and future Army and DoD missions will require autonomous robotic systems for supply missions, information collection, decision aids, and warfare support. Yet, there is still a long way to go to create a vehicle that can drive autonomously with the same abilities as a human. The recent DARPA Urban Challenge (DUC) also revealed the fragile nature of practical robotic intelligence by repeatedly demonstrating how simple perception mistakes can cascade into catastrophic multi-robot failures. This fragility can be linked to one overarching problem in these systems: the mismatch in the integration of perception and planning.

The goal of this research effort is to develop a unified theory for perception and planning in autonomous ground vehicles with a specific focus on obstacle tracking/identification and on vehicle trajectory planning, so as to enable reasoning and robust planning that is intelligent rather than simply reactive. It is anticipated that this research will lead to the development of both object- and map-centric heterogeneous sensor fusion methods for detection, tracking and identification. These innovations will include the development and use of a probabilistic ground model as well as parts-based computer vision methods in order to improve tracking in cluttered environments. It is anticipated that the investigator will develop human-like driving behaviors using a nonlinear, constrained optimization based path planner; innovations include the incorporation of probabilistic models of the environment into the optimizer, including vehicle and obstacle locations, and obstacle motion. Formal guarantees will be explored for both vehicle stability as well as numerical solutions. The unified theory will be analyzed and verified through a three step process ranging from theoretical analysis to empirically driven simulations, to full sized, robotic test bed validation. This process will both codify the advantages and limitations of the fundamental theory and will provide an opportunity for transitioning the results to the Army and DoD.

VI. DIVISION STAFF

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CHAPTER 12: PHYSICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2010* is to provide information on the programs and basic research efforts supported by ARO in FY10, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the future Soldier. This chapter focuses on the ARO Physics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY10.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research seeking to discover and understand exotic quantum and extreme optical physics. The Division aims to promote basic research that explores the frontiers of physics where new regimes of physics promise unique function. Examples such as ultracold molecules, complex oxide heterostructures, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge of physics must be expanded to enable an understanding of the governing phenomena. The results of these research efforts will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Beyond advancing the world understanding of exotic quantum physics and extreme optics, the research efforts managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries resulting from ARO physics research are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and low-power electronics for decreased Soldier load, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division frequently coordinates and leverages efforts within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. Collaborative efforts with the Electronics Division are also underway with a goal of developing the science of magnetic materials and the engineering of agile radio frequency device concepts. The Physics Division coordinates efforts with the AFOSR and DARPA in pursuit of forefront research advances in atomic and molecular physics, including ultracold molecules and optical lattices. The Division also coordinates certain projects with the National Security Agency (NSA), the Joint Technology Office (JTO), and the Joint IED Defeat Organization (JIEDDO). These interactions promote a synergy among ARO Divisions and impact the goals and improve the quality of the Division's research areas.

B. Program Areas

To meet the long-term program goals described in the previous section, the Physics Division engages in the ongoing identification, evaluation, funding, and monitoring of a variety of research projects. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY10, the Division managed research efforts within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics and Imaging Science, and (iv) Quantum Information Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Atomic and Molecular Physics. The goal of this Program Area is to study the quantum properties of atoms and molecules and advance a fundamental understanding of exotic quantum behavior. When a gas of atoms becomes cold enough, they lose their identity and the gas behaves like a wave rather than a cloud of distinct particles. Accordingly experiments that were once the sole purview of optics become possible with matter: interference, lasing, diffraction, up/down-conversion, and others. This Program Area explores these ideas with an eye toward enabling new opportunities, such as gravitational sensing and ultra-high resolution lithography for future electronics. The specific research Thrusts within this Program Area are: (i) Quantum Degenerate Matter, (ii) Ultracold Molecular Physics, and (iii) Optical Lattices. Ultracold gases can be trapped in a one, two or three dimensional standing optical waves enabling the exploration of novel physics, quantum phase transitions, and mechanisms operative in condensed matter. In optical lattices, one can also create a new "electronics" based on atoms and molecules; however, with statistics, mass, charge, and many additional handles not available in conventional electronics. The Molecular Physics Thrust is distinguished from the Program Areas in the Chemical Sciences and Materials Science Divisions because its focus not on synthesis, but on the underlying *mechanisms*, such as electronic transport, magnetic response, coherence properties (or their use in molecule formation/selection), and/or linear and nonlinear optical properties. While the notion of taking objects held at sub-Kelvin temperatures onto a battlefield may seem irrational, dilute atomic gases can be cooled to nano-Kelvin temperatures without cryogens (like liquid nitrogen or liquid helium). The cooling is accomplished with magnetic traps and lasers. The long-term applications of this research are broad and include ultra-sensitive detectors, time and frequency standards, novel sources, atom lasers and atom holography, along with breakthroughs in understanding strongly-correlated materials and our ability to design them from first principles.

2. Condensed Matter Physics. The objective of this Program Area is to discover and characterize novel quantum phases of matter at oxide-oxide interfaces. Recent studies have shown that interfaces can support quantum phases that are foreign to the bulk constituents. Furthermore the bond angles and bond lengths in complex oxides are controllable at interfaces. In general the interface provides a mechanism for potentially controlling lattice, orbital, spin and charge structure in ways that are not possible in bulk, single phase materials. If these degrees of freedom can be engineered in ways analogous to charge engineering in semiconductors, it will present new opportunities for the development of advanced technologies utilizing states beyond just charge. This Program Area also involves research in other material systems that exhibit many-body effects, including synthetic assemblies simulating lattice models. In general discovering, understanding, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technological paradigms. Nanometer-scale physics, often interpreted as a separate field, is also of interest as confined geometries and reduced dimensionality enhance interactions between electrons leading to unusual many-body effects. A critical component for gaining new insights is the development of unique instrumentation and this program supports the construction and demonstration of new methods for probing and *controlling* unique phenomena, especially in the studies of novel quantum phases of matter. Further structures and assemblies exhibiting unique phenomena may require unique synthesis techniques. These range from biological assembly to virtual structures, such as optical lattices. Establishing such techniques for the fabrication or simulation of condensed matter systems are of interest when they provide access to novel quantum phenomena that are not otherwise readily obtainable.

3. Optical Physics and Imaging Science. The goal of this Program Area is to explore the novel manipulation of light and the formation of light in extreme conditions. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research Thrusts within this Program Area are: (i) Negative Index Materials (NIMs), (ii) Transformation Optics, and (iii) Extreme Light.

Negative index materials (NIMs) are artificially fabricated materials whose collective response to light culminates in backward refraction. This program has a particular interest in the development of NIMs that are functional at visible wavelengths and some success has been achieved in this area. Advances have led to research in transformation optics, in which the index of refraction (both positive and negative) of optical materials, is a controllable function of position and possibly time. Possible applications include sub-wavelength imaging, flat or conformal optics, cloaking, and light collection. The Extreme Light Thrust involves investigations of ultra-high intensity light, light filamentation, and femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reactions and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation. Short, intense pulses self focus in the atmosphere until the intensity reaches the breakdown value where nitrogen and oxygen are ionized, creating a plasma. This new form of radiation creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications of these pulses include imaging through opaque materials, laser pulse modulation, and "observing" electron dynamics.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation and in secure communication. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Communication, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms, decoherence mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum computation entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Computation and Communication Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

C. Research Investment

The total funds managed by the ARO Physics Division for FY10 were \$67.4 million. These funds were provided by multiple funding agencies and applied to a variety of Program Areas, as described here.

The FY10 ARO Core (BH57) program funding allotment for this Division was \$5.1 million. The DoD Multi-disciplinary University Research Initiative (MURI), and Defense University Research Instrumentation Program (DURIP) provided \$6.7 million to programs managed by the Division. The Division managed \$8 million provided by the Defense Advanced Research projects Agency (DARPA), and \$45 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and the Small Business Technology Transfer (STTR) programs provided \$1.8 million for awards in FY10. Finally, \$0.8 million was provided for awards in the Presidential Early Career Award for Scientists and Engineers (PECASE) program and the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) outreach program.

II. RESEARCH PROGRAMS

ARO participates in the identification and management of projects within many research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY10 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) research program. The primary goal of the Core program is to support high-risk, high-payoff basic research projects. These projects include single investigator (SI) grants, Short Term Innovative Research (STIR) grants, and conferences and workshops (the largest of which are discussed in the following section). Research projects are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research efforts. Selected projects are discussed later (see Sections III-V) with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

B. Workshops and Symposia

1. Complex Oxide Interfaces Workshop (Charlottesville, VA; 23-24 August 2010). The purpose of this workshop was to assess the progress and future research directions of fundamental research in emergent phenomena at complex oxide interfaces. While many of the lessons learned in semiconductor interfaces are being applied to complex oxide interfaces, it is becoming clear that the physics and chemistry prevalent in semiconductors is not the same as in oxides. The workshop brought together academic leaders in the field to discuss phenomenological and *ab initio* theory, epitaxy, defect modeling and mitigation, and materials characterization to include scanning tunneling electron microscopy, x-ray spectroscopies, optical studies and transport. The information and discussions shared at this workshop resulted in renewed interest in pursuing research directed toward the advancement of this field.

C. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. New Imaging Methods. This MURI began in FY05 and was awarded to a team led by Professor Robert Boyd at the University of Rochester. The objective of this research is to investigate new imaging methods that can be used to analyze various materials.

Recent advances in quantum optics and in quantum information science have created the possibility of entirely new methods for forming optical images with unprecedented sensitivity and resolution. This research focuses on exploring quantum new methods for image formation enhanced by quantum mechanics (or possibly by exploiting previously-undiscovered analogies with quantum mechanics). Four specific approaches for quantum imaging are being explored: (i) optical coherence tomography, in which quantum effects are used to increase the axial resolution of the imaging system and are used to extract useful information regarding the dispersion of the material, (ii) ghost imaging, in which one can use coincidence techniques to form images using photons that have never interacted with the object to be imaged, (iii) laser radar, for which a noise-free quantum preamplifier

might be developed with increased detection sensitivity, and (iv) lithography, where the use of quantum-entangled photons can enable one to write structures at a resolution exceeding that imposed by classical diffraction theory.

2. Advancing Fundamentals in Optics. This MURI began in FY06 and was awarded to a team led by Professor Vlad Shalaev at Purdue University. The objective of this MURI is to advance the field of optics through the construction of negative-index materials (NIMs) operational at visible wavelengths.

In current optics technology, light refracts (bends) as it passes from one material to another. By curving a surface, such as a lens, refraction is used to focus light. Unfortunately this process loses some of the information contained within the light. As a result current lenses, such as those used in a microscope, essentially prevent the user from viewing objects smaller than the wavelength of visible light (*i.e.*, limited to about 0.5 micrometers). NIMs offer the possibility of developing a perfect lens that in principle could allow an experimenter to see objects at a nanometer scale - much smaller than the diffraction limit. These lenses could be used for sensors, microscopy, and for production of ultra-resolution lithographic structures. NIMs can be designed through the use of metamaterials (artificial materials engineered to provide specific properties not available in naturally-made structures) or by the construction of photonic crystals. The team has already produced NIMs that function at both infrared and visible wavelengths. While this MURI is nearing its final year of funding, the overarching goals of this program will be addressed by a new MURI led by Professor David Smith, with Professor Vlad Shalaev contributing as a co-PI (see Subsection 7: Transformation Optics - Exploring New Frontiers in Optics).

3. Quantum Many-body Physics for the Study of Biological Mechanisms. This MURI began in FY07 and was awarded to a team led by Professor Rick Kiehl at the University of California, Davis. The objective of this research is to employ biological mechanisms to study novel quantum phenomena.

Numerous novel quantum phenomena resulting from many-body interactions are present in condensed matter systems with a length scale at or just beyond the reach of current lithographic technology (<10 nm). Biological mechanisms, however, naturally operate on such length scales. The specific goals of this program are: (i) to use studies of biological assembly of individual and multiple nanostructures for systems exhibiting quantum many-body phenomena and to do so in such a way that the phenomena are accessible, and (ii) to demonstrate the systematic study of such phenomena. These goals will be pursued by research involving (a) DNA and protein-based directed assembly of nanostructures, (b) chemical modification of the nanostructure surfaces for protection of the inorganic core and for binding to biological macromolecules, and (c) transport and spectroscopic studies of nanostructure arrays and devices exhibiting quantum phenomena. It is anticipated that the MURI will open a new avenue to study many-body phenomena and will accelerate research toward a fundamental understanding of these phenomena. Results from this MURI are expected to lead to new opportunities for technological development based on novel quantum phases of matter that are as-of-yet inaccessible.

4. Record-fast Laser Pulses for New Studies in Physics. This MURI began in FY07 and was awarded to a team led by Professor Zenghu Chang at Kansas State University; however, Professor Chang is now a co-PI for this project due to his transition to the University of Central Florida. The objective of this research is to investigate methods for generating extremely rapid laser pulses.

Attosecond (one quintillionth of a second or 10^{-18} s) laser pulses are a new regime and are expected to revolutionize physics and technology just as the femtosecond (one billionth-billionth of a second, or 10^{-15} s) era did. Just as the previous epoch ushered in a new generation of physics and engineering, attosecond science is expected to provide the foundation for unprecedented achievements, ranging from precision laser surgery to quantum molecular control. Such short pulse generation is now possible due to the recent attainment of record high laser intensities (1,022 W/cm^2) coupled with breakthroughs in chirped-envelope phase control. The researchers are attempting to develop attosecond pulses that approach the atomic timescale (~25 attoseconds), which will provide the first opportunity to monitor, understand, and eventually control the molecular electronics underlying any physical, chemical and biological system. Potential future Army-relevant applications include gas-phase reaction studies (*i.e.*, combustion), molecular electronics in nanoparticles (*e.g.*, nanotubes, nanorods, quantum dots), and electronic coherence studies in solids (*e.g.*, for building faster electronic devices). The vast spectrum in the Fourier decomposition of these ultrashort pulses demonstrates that they contain components above the plasma frequency for any substance and will, therefore, propagate through solid materials. This property provides the basis for a new kind of imaging, with applications ranging from weapon detection to uncovering defects in materials.

5. Conversion of Quantum Information among Platforms. This MURI began in FY09 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland. The objective of this MURI is to explore the conversion of quantum information from one form to another.

Since the inception of research in quantum information, a number of platforms have been explored to implement quantum information: trapped ions, ultracold atomic gases, semiconductor quantum dots, superconductors, and others. Each of these systems has a unique advantage while also suffering disadvantages in other areas. For example, trapped ions are relatively easy to manipulate and are readily isolated from the environment. However they cannot be readily scaled up to the size necessary for practical applications. Semiconductors are perfect for that, but the quantum information is too quickly lost to the surrounding material for a practical computation to occur. To address these matters, the MURI is considering the potential for converting quantum information from one platform to the other without losing the quantum nature of the information. In particular the intra-conversion of information between atomic systems, solid state systems, and optical systems will be explored. If the best of each platform can be combined and the detrimental problems avoided, then the development of quantum information capabilities will be accelerated. The advent of a quantum computer will provide solutions to problems that are computationally intractable on conventional computers, impacting resource optimization and improved logistical support.

6. Harnessing Electronic Phenomena at Oxide Interfaces. This MURI began in FY09 and was awarded to a team led by Professor Susanne Stemmer at the University of California, Santa Barbara. The objective of this research is to investigate the unexpected electronic effects found to exist at the interfaces of certain crystalline oxides.

Recent studies have shown that carefully designed and grown interfaces between different crystalline oxides can lead to electronic phenomena at that interface that are foreign to the oxides that form it. These studies have suggested the potential for a new type of electronics technology; therefore this new MURI aims to determine if these effects can be designed and controlled. The research focuses on the Mott transition - a metal-to-insulator transition that results from electron-electron repulsion. The objective is to design and control the oxide-oxide interface as a new approach to understanding, predicting and controlling the Mott metal-insulator transition and the associated electronic phenomena. The electronic energy states that determine the character of the material are tied to the metal-oxygen atom distance in the crystal and the crystal symmetries. Accordingly the team will construct alternating layers of a material containing a known Mott metal-insulator transition with an insulator that will affect the bonding distances and symmetry of the adjacent Mott material. The ability to control this transition may lead to new options for enhancing logic, memory and other technologies important for advanced computational capabilities.

7. Transformation Optics - Exploring New Frontiers in Optics. This MURI began in FY09 and was awarded to a team led by Professor David Smith at Duke University. The objective of this research is to explore new frontiers in optics made possible by NIMs.

Advances in NIMs, many of which were developed by the MURI team led by Professor Vlad Shalev (refer to Subsection 2: Advancing Fundamentals in Optics), have led to a new field in optics termed transformation optics. By combining the negative refraction of NIMs with an index of refraction that varies spatially and temporally, optical materials can be designed to have properties not possible with conventional optics. This MURI began to explore this new frontier in physics and the research team includes Professor Vlad Shalev as a co-PI. The MURI team will investigate methods of controlling light by design, routing it where conventional optics cannot. For example with transformation optics, light of a particular wavelength can be bent around an object rendering the object invisible at that wavelength. This has already been demonstrated in the microwave band but has not yet been shown at the wavelengths of visible light. The second objective is the development of a flat hyperlens: a lens that is flat on both sides and not only magnifies but also resolves nanometer-scale features. This lens could provide a resolution at least an order of magnitude beyond the diffraction limit of conventional optics. Not only can transformation optics be used to bend light around an object but it can also be used to bend light toward an object. The third major objective is to design materials accordingly such that light from all directions is concentrated on a single detector. These concentrators could revolutionize optical sensors and solar energy collection as its omnidirectional nature eliminates the requirement of moving parts.

8. Atomtronics: Investigating Atom-based Physics. This MURI began in FY10 and was awarded to a team led by Professor Ian Spielman of the University of Maryland. The objective of this MURI is to explore and understand the concepts of atom-based physics, beginning with the rich and fundamental physics discoveries already revealed with cold atoms systems and to investigate the concepts required for future device applications.

Atom-based physics studies (atomtronics) are analogous to, but will go beyond, the fundamental 20th century studies regarding the properties of electrons (*i.e.*, electronics) that enabled the electronics revolution. Solid-state electronics, heralded by the transistor, transformed both civilian and military culture within a generation. Yet there is only a single kind of electron: its mass, charge and spin (and thus quantum statistics as well) are unalterable. Atoms on the other hand, come with different masses, can have multiple charge states, and have a variety of spin and other internal quantum states. Accordingly studies in atomtronics aim to understand an atom-based physics rather than electron-based device physics. Breakthroughs in cold atom physics and degenerate quantum gases presage this new kind of device physics. That cold atom science has resulted in atomic analogies to other technologies, such as optics and lasers, suggests that the same may be repeated with electronics. Very good analogies of solids and junctions can be made with trapped atoms. It is now well-known how one, two and three dimensional structures with essentially any lattice geometry can be formed in cold, trapped atoms. Presently a few theory papers are pointing the way to simple devices.

The most apparent, but not necessarily the only approach to atomtronics, is through optical lattices, where Bloch's theorem holds. Band structure is the first basis on which physicists understand traditional (electronic) metal, insulator, and semiconductor behavior. Interaction and disorder modify this and exploration of Mott-like and Anderson-like insulators and transitions are envisioned as well. Doping can be mimicked by modifying atoms in certain wells or by locally modifying the lattice potential, which can be done with additional optical fields. Such defects could be deeper or shallower wells, or missing, or could be additional sites. Recent breakthroughs involving three dimensional optical lattices and the loading of atoms into lattices with reasonably long lifetimes have set the stage for atomtronics.

Atomtronics researchers are focused on two key themes devices and connections. The envisioned analogs to devices can be described as those that perform actions under external control and those that are cascadable. The researchers will explore spin-orbit coupling in atomic systems in an effort to exploit new degrees of freedom in "spintomic" devices as well as novel reversible logic via cascadable spintomic gates. In addition researchers will investigate far from equilibrium regimes, which is not possible in condensed matter systems due to the residual phonon interactions at finite temperatures. The second theme centers on connections and is split between analogs to electronics and novel interfacing. The research team will use the superfluid properties of ultracold atoms confined in rings to create circuits. These small circuits will interact with lasers to demonstrate an analogous SQUID device. Finally the researchers will explore novel interfacing by trapping atoms with evanescent waves along ultrathin optical fibers. It is hoped that this technique will allow several devices to be coupled while remaining isolated from the environment.

D. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY10.

E. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as was described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Complex Oxide-based Bolometry. A Phase II STTR contract led by Agiltron, Inc., is developing a complex oxide-based microbolometer focal plane array. Microbolometers are devices used to detect energy in the form of infrared radiation that is emitted from organisms or the environment. These devices are used as detectors in thermal cameras and are usually constructed using a grid of vanadium oxide or amorphous silicon heat sensors above a grid of silicon. Unfortunately these materials have a limited sensitivity; therefore below a certain threshold, they cannot detect low-energy infrared emissions. Current state-of-the-art uncooled infrared bolometers suffer from 1/f noise which leads to pixel-to-pixel non-uniformities in focal plane arrays (FPAs). An improvement in 1/f noise is paramount. A larger thermal coefficient of resistance (TCR) would also benefit the

technology. Bolometer technology typically relies on VOx or amorphous silicon but other materials have been considered. Oxides such as colossal magnetoresistive (CMR) manganites or others exhibiting metal-insulator transitions have shown promise. Recent results indicate that these materials provide low noise and high TCR characteristics. While these results are promising, noise characteristics depend on more than just the material; device fabrication steps and bolometer design including detector area, bandwidth and integration time all play a role. If successful these microbolometers will significantly improve the sensitivity of thermal imaging in applications of interest to the Army.

2. Metallization Techniques for Microwave Devices. A Phase II STTR contract led by US Ferroics, Inc., is developing metallization techniques suitable for radio frequency (RF) technologies. Oxide-based radio frequency (RF) components have many advantages over more traditional approaches as they are small, reliable and continuously tunable. However there are also disadvantages to oxide-based components. The two most significant problems limiting the adoption of this advantageous technology are loss and temperature instabilities, especially at higher frequencies. To date efforts toward solving these problems have focused almost entirely on optimizing the oxide material itself and much progress has been made. Little attention has been given to optimizing the electrode materials, the metal/oxide interface or the metallization process, all of which are inter-related. Given that the conductors provide the dominant loss mechanism, including insertion loss for these devices, this is a critical design factor for high frequency components. If this research is successful, understanding how the electrodes specifically effect the device operation can enable the design of components and processes optimized for military and commercial markets.

3. Ultraviolet and Blue Compact Laser Sources for Scalable Quantum Computing. A Phase II STTR contract led by AdvR Inc., is designing and developing an innovative compact ultraviolet (UV) laser source that would enable quantum computing and broader sensor technology. Many trapped ion systems used for qubits require UV or blue laser sources for their operation. The UV sources currently available are costly, bulky, and difficult to use outside of a carefully controlled research environment. As a result, these UV sources impede the development of systems with more qubits (quantum bits), a necessity for quantum computing applications. Trapped ions represent one of the very promising avenues for scalable quantum computing. Typical wavelengths needed for cooling, optical pumping, and qubit operations are in the 200-400 nm range. These wavelengths are also very useful for chemical and biological sensing. CW power requirements are in the range of a few milliwatts along with narrow band operation (*i.e.*, a few MHz). Output modes should be close to TEM00, with good pointing stability and low power fluctuations (*i.e.*, a few percent). Currently complicated frequency doubled or quadrupled systems involving large lasers are used. Lenses and mirrors outside the vacuum chamber are used to steer the laser beams. These techniques are satisfactory for the early experiments involving a few ions (qubits) but are too complicated to scale to larger systems. Through a previously-completed Phase I contract, periodically-poled materials were demonstrated to upconvert readily available diode lasers to the blue and UV wavelengths. In this Phase II project, researchers aim to finalize the design and build prototypes of the laser source. If successful this research will lead to the development of commercially-available, simple, compact, narrow-band UV laser sources. These lasers will enable the scale-up of trapped ion quantum computing, a development that can provide the Army with increased computational capability for solving difficult problems, for information assurance, and for improved data integrity.

F. Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) and Tribal Colleges and Universities (TCU) – New Starts

The goals of the HBCU/MI and TCU programs are to enhance the research capabilities and infrastructure at minority institutions and to increase the number of under-represented minority graduates in scientific disciplines. A more detailed description of the history and objectives of these programs is available in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Investigating Carbon Nanotubes for Optoelectronics. The objective of this HBCU project, led by Professor Igor Bondarev at North Carolina Central University, is to carry out theoretical studies of electronic band structure and excitonic effects in pristine and atomically doped carbon nanotubes.

Carbon nanotubes, one of the many allotropes of carbon, have unique electronic and optical properties, primarily due to the one dimensional nature of their structure. While research elsewhere progresses toward isolation of

nanotubes of specific chirality and characteristics, this effort focuses on the extent to which the optical and electrical properties of nanotubes can be controlled. One of the several aspects of this research includes the comparison of isolated and bundled nanotubes. When not wrapped with organic ligands, nanotubes are interminably bundled due to Van der Waal forces. In addition to the standard electronic band structure that will be calculated using density functional theory, exciton-plasmon and exciton-polariton effects will be studied with quantum electro-dynamics. These latter effects strongly influence the optical properties of the nanotubes. If the sum of these interrelated effects is understood and controllable, nanotubes may serve to enhance battlespace awareness and power and energy through sensors and energy conversion and storage.

2. Expanding the Library of Optoelectronic Materials. The objective of this HBCU project, led by Professor Marvin Wu at North Carolina Central University, is to fabricate and characterize III-V and II-VI nanostructures.

This effort aims to create advances in materials suitable for future photovoltaic and other optoelectronic applications. The ultimate goal of this project is to expand the number of useful materials available for optoelectronic structures. The research team is using laser ablation to synthesize III-V and II-VI nanostructures with varying composition and doping. The research involves a systematic investigation of Chalcopyrite and ternary and quaternary semiconductors to relate size, composition and doping levels to optoelectronic properties. Photoluminescence is being used as a preliminary characterization tool. Concurrently theoretical studies are being conducted with the intent of developing predictive scientific modeling capabilities.

G. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY10.

H. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY10, the Physics Division managed nine new DURIP projects, totaling $1.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO, including studies of ultracold Fermi gases, ultracold polar molecules, magnetic nanostructures, transformation optics and quantum information science.

I. DARPA Information in a Photon (InPho) Program

The goal of the DARPA InPho Program is to pursue the basic science and the associated unifying physical and mathematical principles that govern the information capacity of optical photons, exploiting all relevant physical degrees of freedom. Important outcomes of this program include (i) the rigorous quantification of photon information content for communications and imaging applications in both the classical and quantum domains, (ii) novel methodologies to maximize the scene information that can be extracted from received photons in next-generation imaging/sensing platforms, and (iii) novel methodologies to maximize the information content of transmitted/received photons in next-generation communication systems. This program builds upon ARO-supported advances in quantum information and optics and is expected to further advance the fields while also exploring opportunities for applications in sensing and communications.

J. DARPA Optical Lattice Emulator (OLE) Program

The DARPA OLE Program seeks to develop methods to exploit the control of, and universal properties of, ultracold atoms confined in optical lattices to simulate the quantum properties of bulk materials. A better understanding of the properties of novel artificial materials can be made possible using exquisite control of the microscopic state and interactions of the atoms. Furthermore specific phase transitions can be simulated to complete our understanding of the fundamental processes that governs high-temperature superconductivity. This program was motivated in large part by the Physics Division and compliments many ARO-supported research efforts in ultracold gases, providing theoretical and experimental synergy to the Core program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies the fundamental research discoveries, results, and accomplishments that originated from research efforts funded and/or monitored by the Physics Division.

A. Laser Cooling of Molecules

Professor David Demille, Yale University, Single Investigator Award

The objective of this research is to develop techniques for trapping large samples of polar molecules and cooling them to the μK range. The researcher recently achieved a considerable breakthrough in the ability to cool and trap molecules that could enable revolutionary new capabilities in sensors and computers. This important achievement follows two decades of research in making and exploiting ultra-cold atoms. The creation of ultra-cold atoms (of a single element) in the 1980s demonstrated that when a gas of atoms becomes cold enough, they lose their identity and behave like a wave rather than a cloud of distinct particles. This discovery opened the door to powerful new areas in basic science research and many DoD applications, as experiments and applications that were once only possible with light (*i.e.*, optics) became possible with matter. Given the enormous civilian and military contributions made possible by the laser cooling of atoms, extending this research to the realm of molecules has become a holy grail of sorts in the physics community.

In contrast to atoms, molecules exist in specific rotational and vibrational states. This complex internal structure prevents a simple extension of atomic laser-cooling to the molecular realm; however, this increased complexity can also provide scientific opportunities not possible with atoms. For example, molecules cooled near absolute zero can enable phenomenally exquisite control over chemical reactions, opening the door to the future development of new functional materials with uses ranging from power generation to armor.

Along with the recent demonstration of ultracold quantum chemistry, another critical experiment was performed demonstrating a new cooling technique for diatomic molecules. In a recent article[1], Professor DeMille and his team have demonstrated the ability to directly laser cool an entire class of diatomic molecules. The researchers were able to implement a clever scheme that prevented the molecules from spontaneously relaxing into dark states, which allowed cooling of molecules to the hundreds of μK with only three cooling lasers (see FIGURE 1).

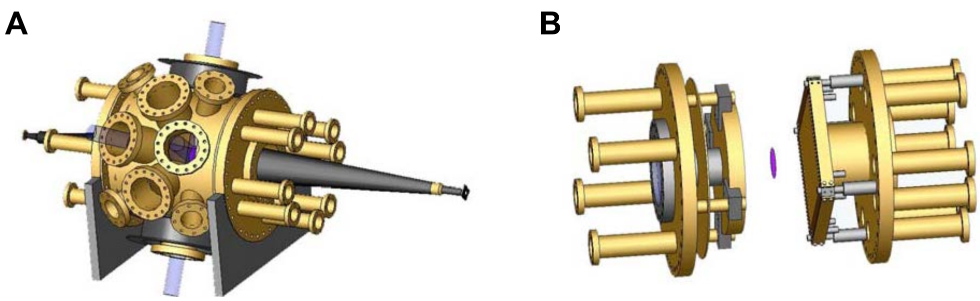

FIGURE 1

Schematic of the ultra-high vacuum magneto-optical trap (MOT) chamber used for the successful laser-cooling of molecules. The schematics reveal (**A**) the full chamber geometry, including MOT coils and laser beams, as well as feeds for inserting and detecting microwave power in the cavity, and (**B**) a view of the interior of the chamber, showing the cavity geometry and various mounting fixtures. The potential trap volume is illustrated by the purple ellipsoid at the center of the figure.

To achieve laser cooling of the SrF molecules the researchers utilized, remarkably, only three cooling lasers λ_{00} = 663.3 nm, λ_{10} = 686.0 nm, and λ_{21} = 685.4 nm. This experimental approach allowed the investigators to directly cool a diatomic molecule to a few mili-Kelvin and demonstrated as a proof of principle a technique applicable to several similar molecules. This latest discovery is notable because directly cooling molecules was once considered impractical due to the complexity of their rotational and vibrational structure. This structure

[1] E.S. Shuman, J. F. Barry, and D. DeMille. (2010). Laser cooling of a diatomic molecule. Nature 467, 820-823.

provides many possible relaxation channels that make it difficult to obtain cyclic transition, a requirement for laser cooling; however, Professor DeMille has demonstrated a method for achieving this cyclic transition with an unanticipated simplicity and generality.

In addition to the potential materials-development applications previously described, the long-term applications of these fundamental physics advances will extend beyond the opportunities made possible with ultra-cold atoms. For example, ultra-cold molecular interferometry can exceed the precision of ultra-cold atoms, further extending the capabilities of promising applications such as highly-accurate and jam-proof gyros (for navigation), accelerometers (for inertial guidance), and sensors such as magnetometers (mine detection) and gravity gradiometers (remote tunnel/bunker detection) for use by the Soldier.

B. Quantum Gas Microscope

Professor Markus Greiner, Harvard University, DARPA OLE Program

Researchers sponsored through a DARPA and ARO co-managed OLE program have for the first time tracked individual atoms in ultracold gas as they organize from a superfluid to a Mott insulator (MI) state. This research opens up the possibility of an atom-by-atom study of the phase transitions in engineered materials (*e.g.*, to understand the mechanism that gives rise to room temperature superconductivity). By studying the physics of quantum materials and refining and verifying current theories, it is anticipated that current materials can be made more efficient. For instance measuring the local dynamics of the microscopic ensemble can offer insight in how the macroscopic statistical properties emerge. In addition to imaging single atom-single lattice sites, this experiment will control the microscopic arrangement of the atoms and probe it. In particular this research explores the bosonic Hubbard model, specifically at the quantum phase transition from superfluid to Mott insulator state.

A recent experiment by this team utilized overlapping lasers tuned in such a manner as to create a standing interference pattern. This interference pattern, commonly referred to as an optical lattice, has a periodic intensity that attracts and localizes the atoms in a similar manner as electrons in crystal. This approach enables precise control over the intensity of the localization as well as how strongly the atoms interact with each other. By carefully controlling the experimental parameters and observing the resulting behavior of atoms, the researchers can gain important insights into how matter behaves in a crystal, an aspect normally inaccessible because of defects and thermal noise. The researchers successfully adjusted the interaction strength of the ensemble of atoms and monitored the behavior of atoms as they transitioned from the MI state to the superfluid state. At zero temperature, a fixed number of atoms occupy each lattice site representing the MI phase and the atom number fluctuates when this temperature takes a finite value. The team recently discovered[2] that the MI could form small stable islands at finite temperatures. A cooling or transfer of thermal excitations appears to take place at the interface of these island regions with the local superfluid regions surrounding these islands and suppressed number fluctuations. FIGURE 2 displays the quantum gas microscope and data from the MI phase.

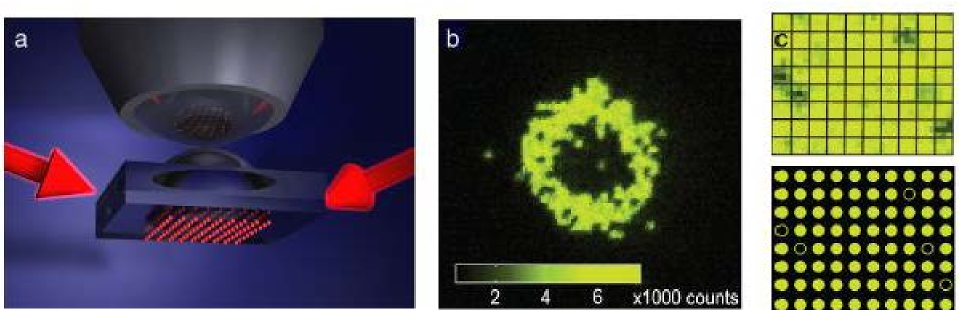

FIGURE 2

Mott insulator (MI) in a quantum gas microscope. (A) The quantum gas microscope, shown in this cartoon, enables high-fidelity single lattice site imaging. The remainder of the figure shows the (B) Mott insulator shell structure with n=1 MI (bright ring), surrounding a n=2 MI core (dark), and (C) a near perfect n=1 Mott insulator.

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[2] W.S. Bakr, J.I. Gillen, A. Peng, S. Fölling, and M. Greiner. (2009). A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice. Nature 462, 74-77.

The researchers were also able to measure the time scale of the MI formation near the lattice sites. The researchers measured the time it took to suppress the atom number fluctuations and found the time to be in the milliseconds. These measurements provide valuable new information regarding the microscopic behavior of electrons in materials across an important phase transition.

In addition to potentially enabling future observations of the d-wave superfluid phase, the quantum gas microscope has many other potential uses. Single-site imaging could also be applied to the study of the spatial correlations of strongly correlated gases. This could lead to a direct measurement of entanglement and be utilized for quantum computing quantum encryption. In addition if the low entropy Mott domains can be carried over to spin models, modeling magnetically ordered states could be directly detected with this single site imaging technique. This would lead to a better understanding of the microscopic ordering of macroscopic anti-ferromagnetic states and this information could prove invaluable for understanding how bulk properties arise from the microscopic conditions and provide a framework for designing novel materials.

C. Two-dimensional Electron Gas Physics in a Complex Oxide

Professor Susanne Stemmer, University of California, Santa Barbara, MURI Award

The objective of this project is to investigate the unexpected electronic effects found to exist at the interfaces of certain crystalline oxides. Understanding two-dimensional quantum phenomena in complex oxides is important both from a fundamental physics perspective and for device applications. For example, confined electron gases in $SrTiO_3$ have recently attracted attention for their potential of combining unique field-tunable, magnetic and superconducting phenomena that cannot be obtained with traditional semiconductor heterostructures. While quantum transport phenomena have been widely investigated in conventional semiconductors, extending these studies to complex oxides has been difficult because the charge carriers in oxides grown by conventional techniques often show too low mobilities.

The researchers have demonstrated that two-dimensional quantum oscillations can be observed in $SrTiO_3$ films that were "delta-doped" with lanthanum. A micrograph of La-doped $SrTiO_3$ demonstrating the superb crystalline quality of these films is shown in FIGURE 3.

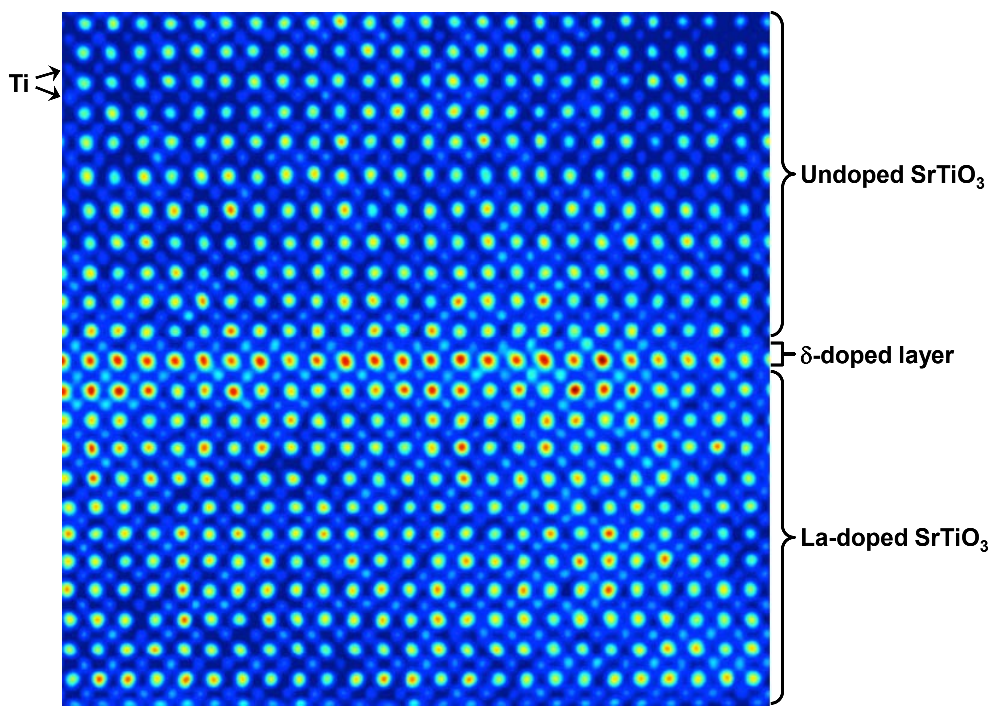

FIGURE 3

Scanning-tunneling electron micrograph of La-doped $SrTiO_3$. This image along the (001) direction clearly shows La and Sr atoms. The Ti sub-lattice is visible as faint light-blue dots.

A prerequisite for this study was the deposition of highly-perfect $SrTiO_3$ layers and excellent control over doping as afforded by new oxide molecular beam epitaxy (MBE) approaches developed by these researchers. The $SrTiO_3$ films grown by MBE were found to have very high electron mobilities – exceeding even those of single crystals. In a metallic system such as a two-dimensional electron gas, the transport characteristics as a function of an applied magnetic field will oscillate with the field strength due to the quantization electron energy. The oscillations for the La:$SrTiO_3$ system are shown in FIGURE 4. The study shows that the electronic structure of quantum confined electron gases in $SrTiO_3$ is inherently much more complex than that of two-dimensional electron gases in conventional semiconductors. In $SrTiO_3$, the sub- bands that form upon quantum confinement are derived from four d-band states near the conduction band minimum of $SrTiO_3$. Despite this complexity, the researchers showed that the quantum oscillations can be modeled quantitatively by recognizing that the magnetic field induced effective spin splitting and Landau level splitting are comparable in magnitude. The results open the way to control quantum phenomena in oxide heterostructures.

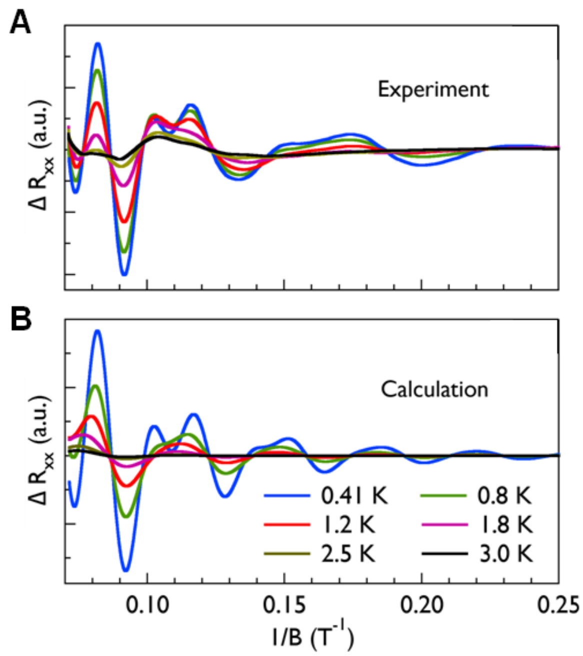

FIGURE 4

Shubnikov-de Haas oscillations of 2D electron gas in δ-doped $SrTiO_3$ layer grown by MBE. The graphs are of (A) experimental data, with the longitudinal resistance shown as a function of the inverse of the magnetic field at temperatures between 0.41 and 3 K, and (B) calculated Shubnikov-de Haas oscillations using a single, spin-split sub-band model. The different periodicities in the experiment and calculation at low magnetic field (right side) indicate that the electron concentration in the sub-band is not constant.

D. Asymmetric Orbital-strain Interactions in Complex Oxides

Professor Jak Tchakhalian, University of Arkansas, Single Investigator Award

The conventional picture of orbital engineering with strain suggests that the dominant ground state orbitals in an epitaxial oxide can be induced with the appropriate selection of lattice mis-match between it and the substrate. Lattice mis-match induces a tetragonal strain that should raise or lower the e_g states relative to the strain-free oxide giving rise to an imbalance in the electron occupancy of the states. This orbital polarization, assumed to be symmetric with strain, should have strong influence over the electronic properties of the materials. Because this conventional picture has failed to explain results in numerous perovskite oxides, this research was conducted to explore the details of the interaction between strain and orbital occupancy polarization.

$LaNiO_3$ (LNO) is a correlated and orbitally degenerate perovskite and is therefore an ideal material for studying this relationship. The LNO *d*-states are occupied with seven electrons with the t_{2g} states filled and a single electron occupying the two e_g states. According to the conventional model, both compressive and tensile strain should split the two e_g states and effect the relative occupancy. LNO was epitaxially grown by pulsed laser deposition on $LaAlO_3$ (LAO) and $SrTiO_3$ (STO). The LAO substrate induces a compressive strain (-1.08%) and

the STO substrate a tensile strain (+1.83%). Because of the natural linear polarization of x-rays from a synchrotron, synchrotron-based X-ray absorption spectroscopy (XAS) is a superb tool to study the orbital polarization between e_g states in crystalline materials. By tilting the sample in the x-ray beam, one can emphasize one polarization over the other. The XAS results and interpretation are shown in FIGURE 5.

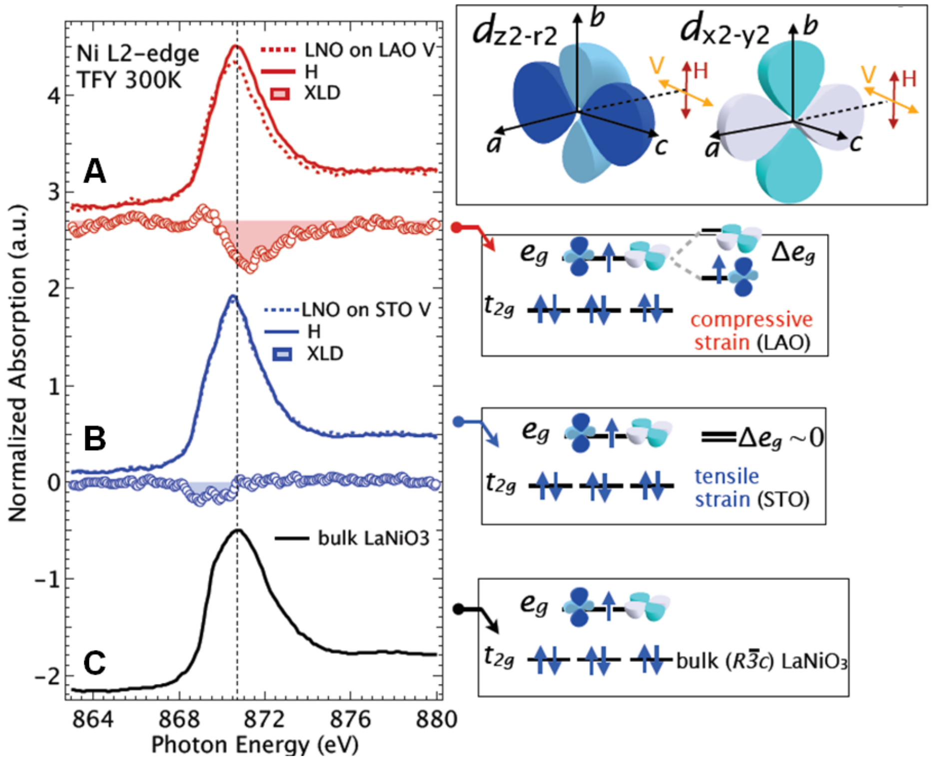

FIGURE 5

Strain-induced orbital polarization in ultra-thin $LaNiO_3$ films. Normalized absorption spectra at the Ni L2-edge taken in the bulk sensitive (TFY) detection mode with varying photon polarization as shown in the legend. X-ray linear dichroic signals (filled symbols) for films under (A) tensile (blue) and (B) compressive (red) strain, on $SrTiO_3$ and $LaAlO_3$ substrates, respectively. Label H denotes a polarization vector along *a* x *b* or the epitaxial plane, whereas V denotes polarization aligned along the *c*-axis. The black curves in (C) represent the bulk (ceramic) $LaNiO_3$ data. Right: Schematic orbital level diagram for bulk $LaNiO_3$ and the anticipated strain-induced orbital polarization effect on the e_g doublet. The XLD data suggests the model is violated for the tensile strain state (on $SrTiO_3$) as indicated by Δe_g ~0 splitting of the Ni^{3+} e_g orbital levels.

Compressive strain was found to split the e_g states, as expected. However tensile strain was found to have no measurable effect on the states. A density function theory study of the structure of this system under strain was undertaken to explain the origin of this asymmetry. For the compressive strain induced by the LAO substrate, the calculations revealed that the in-plane and out-of-plane Ni-O bonds are smaller than anticipated by the conventional model. It turns out that the flexibility of the perovskite structure, having a octahedron inscribed within a pseudo-cube, allows bond bending to play a role in elastic strain accommodation in addition to the bond stretching assumed by the conventional model. Furthermore when the STO substrate induces a tensile strain, the picture is even more unique. The tensile strain induces a breathing structural distortion with a 3D checkerboard pattern of large and small NiO_6 octahedra (see FIGURE 6).

This study demonstrates another aspect of complex oxide physics for which conventional wisdom does not apply. By investigating these fundamental aspects of complex oxide heterostructures, it is hoped that a technique for engineering complex oxide properties for unique electronic and optical technologies can be developed.

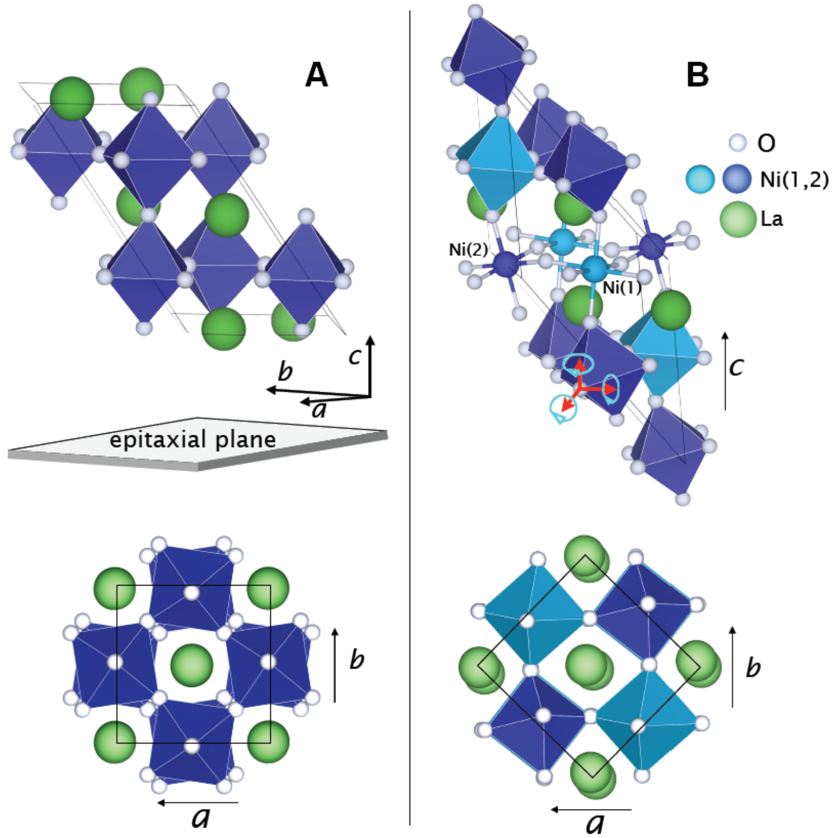

FIGURE 6

First-principles calculated crystal structures at the experimental lattice constants. (A) The left images show compressive strain on $LaAlO_3$: the space group is *C2/c*, with a = 9.415 Å, $b = c$ = 5.536 Å, and a monoclinic angle of 124.7°. The bulk $LaNiO_3$ crystal structure (not shown) possesses a higher symmetry due to a trigonal axis along the body diagonal that is removed by the epitaxial constraint. (B) The images on the right illustrate tensile strain on $SrTiO_3$: the space group is $P2_1/c$, with $a = b$ = 5.515 Å, and c = 9.439 Å, and a monoclinic angle of 125.8°. Two symmetry unique octahedra $Ni(1)O_6$ and $Ni(2)O_6$ are shown in different shades.

E. Plasmonic Resonance: Negative Index Materials and Beyond: the Spaser

Professor Vladimir Shalaev, Purdue University, MURI Award

The objective of this MURI is to develop optical materials, NIMs, that exhibit a negative index of refraction in the visible and near IR region of the spectrum. One of the hallmark claims of NIMs is the ability to image below the wavelength of light. This has been successfully demonstrated for the case of a NIM cylindrical lens and future research will focus on accomplishing this using a flat lens. The successes in NIMs are partly due to the ability to make metamaterials with negative indices. This is accomplished, for example, by embedding nano-rods of gold or silver into dielectric materials. Due to the increase of the ensuing magnetic permeability, NIMs can now be made in the visible spectrum.

The most essential physical mechanism underlying the operation of these metamaterials is the plasmonic responses of the nano-conductors. For certain shapes, plasmon resonances may be maintained that are tuned by the size and boundary conditions of the sample. The goal is to use gain to overcome the inherent loss due to resonant absorption. Experimental research at Purdue University, a partner of the MURI team, successfully employed surface plasmon amplification by stimulated emission of radiation (SPASER) to create the world's tiniest laser: the spaser-based laser (see FIGURE 7). Although the MURI team did not originally aim to develop this unique laser, the high-risk, high-payoff research led to this serendipitous development based on the negative-index materials focus of the MURI.

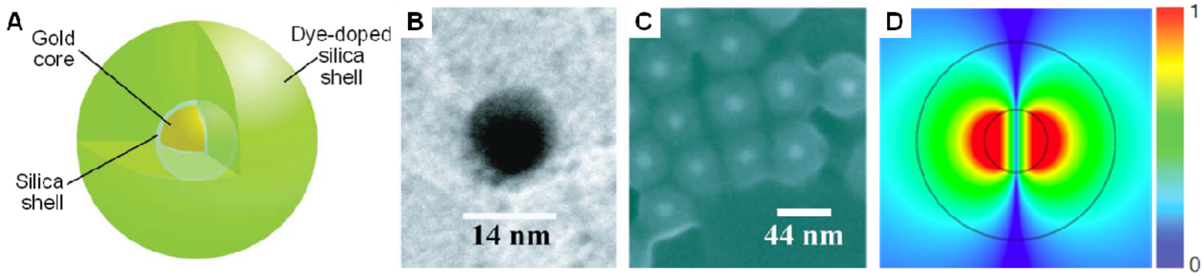

FIGURE 7

The spaser. The figure displays (**A**) a schematic of the metamaterial, which comprises a gold sphere surrounded by a dye-doped silica shell that acts as a gain medium to control the wavelength of emitted light, (**B**) a transmission electron micrograph of the gold core, (**C**) a scanning electron micrograph of a collection of spacers, and (**D**) the spacer mode shown in false color with the field strength color scheme shown to the right.

The spaser consists of a 14-nm diameter gold core enclosed in a silica shell surrounded by an OG-488 dye-doped silica shell that acts as a gain medium. Although conventional lasers can be no smaller than the half the wavelength of light, the gold core is more than an order of magnitude smaller. The reason the spaser functions is because, while electromagnetic waves cannot be constrained to such a small size, plasmonic oscillations (*i.e.*, electronic oscillations) are constrained and excite the optically-active shell. Thus when optically pumped, the spaser emits light of wavelength 525 nm, rightfully earning its moniker as the world's smallest laser. The investigators found that the onset of stimulated emission as the emission curve begins to rise just after the knee in the curve (see FIGURE 8).

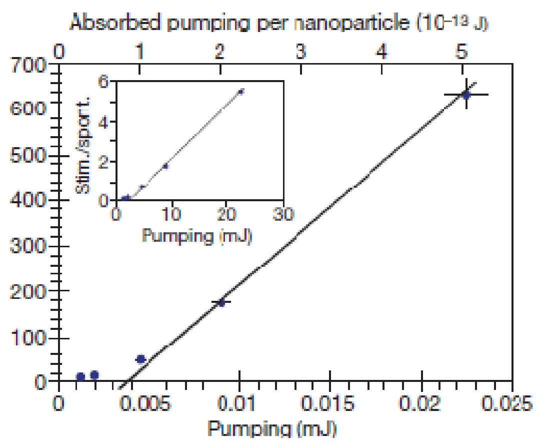

FIGURE 8

Spaser input-output curve. Note the onset of stimulated emission at 0.005 mJ.

This astounding triumph is not only valuable in its own right, but has shown that gain can overcome loss, an important achievement when dealing with NIMs that operate near resonance. Spasers created using these 44-nm nanoparticles may be a critical component for potential future technologies based on revolutionary fast and small "nanophotonic" circuitry - circuits based on movement of light instead of electronics. The future development of nanophotonic circuits will require a laser-light source, which could be provided by spacers since existing lasers cannot be made at the small size required for integration into electronic chips. The spacers may also enable the switching speed of communication systems to be increased by 100-fold. This research could also enable optical computing, with an impact similar in significance as transistor was for electronics.

F. Attosecond Laser Pulses

Professor Shuting Lei, Kansas State University, MURI Award

The objective of this research is to investigate methods for generating extremely rapid laser pulses for potential use in studying very fast phenomena. Ultrafast laser physics has developed over the decades from nano to pico

to femto and now attosecond (10^{-18} s) pulses. The push to achieve attosecond pulses requires new optical sources as well as new measuring techniques. The team starts the process by focusing an intense IR beam into a stream of atoms (see FIGURE 9).

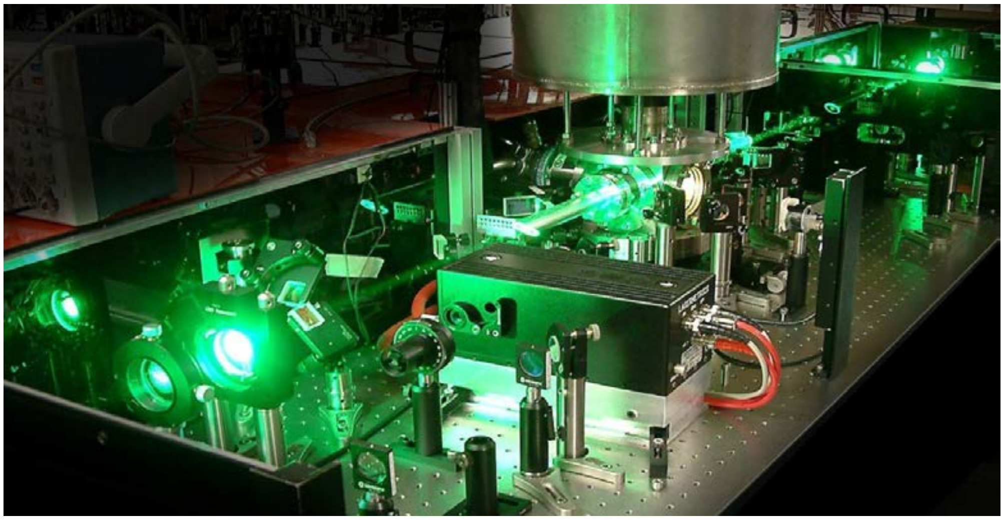

FIGURE 9

Attosecond laser. This laser apparatus was used to generate the attosecond pulses and is housed at Kansas State University.

The high intensity light leads to nonlinearity and results in a train of soft x-ray pulses. The ingenious scheme pioneered by co-PI Prof. Zhengdu Chang (University of Central Florida) was to create two such beams slightly out of phase and with opposite circular polarization. When combined, for the instant the polarizations align, the field can rip an electron from an atom and with the second part of the pulse, slam it back to the parent atom in a process called electron whiplash. This process created a single attosecond pulse.

The investigators have created pulses as short as 120 attoseconds and have most recently created a pulse that has an energy spectrum consistent with a 16 attosecond pulse. The team is attempting to verify that this is a true 16-attosecond pulse. One of the obstacles the team is facing is the worldwide lack of equipment that can measure such fleetingly small times. Nevertheless they are trying to develop new kinds of streak cameras and other ultrafast equipment that can capture the minuscule times involved in the as research. A related problem is the stabilization of the absolute, or carrier, phase of the pulse. Professor Gerhardt Paulus, a team member from Texas A&M, has made great strides in phase stabilization and the team now predicts that they are on the brink of measuring down to 25 attoseconds. The ability to create attosecond pulses enables new areas of basic research, such as improved analyses of the reaction dynamics of chemical reactions. In addition these advances herald a new range of potential long-term applications, such as remote sensing using attosecond-enabled advances in spectroscopy and quantum control.

G. Demonstration of Fast Single-photon Source Using Quantum Dots

Professor Jelena Vuckovic, Stanford University, Single Investigator Award

Sources of single photons on demand are critical for quantum information processing as well as for fundamental studies of light-matter interactions. To achieve indistinguishability of output photons (as is required for quantum computing applications), optical excitation is necessary. The PI and her research group have previously demonstrated the required step of strongly coupling a quantum dot with a photonic crystal cavity. In these studies, the optically triggered quantum dot single photon sources have been excited by bulky, expensive lasers (typically Ti:sapphire), and their communication rate has been limited by the laser repetition rate to around 80 MHz. In addition the quantum dot emitters used in such sources have had output wavelengths that are incompatible with telecommunication systems (typically <1000 nm), which makes the interfacing of such devices with existing optical communications infrastructures difficult.

During FY10 the PI and her research group have achieved the next significant step in this research by demonstrating a practical solution for a quantum dot-cavity, based single photon source triggered at 300 MHz by a telecommunications wavelength (~1500 nm) laser. The excitation is achieved by using a compact telecommunication laser whose output is modulated at 300 MHz with an external off-the-shelf electro-optic modulator (see FIGURE 10). The excitation beam is coupled to a photonic crystal nanocavity (in which a quantum dot emitter is also embedded), which recirculates it, and generates the second harmonic (light at ~750 nm wavelength) that excites the quantum dot. Second harmonic generation is resonantly excited by the cavity and the experiments have shown that it can be generated with only several nW of the coupled input powers. This single-photon generation speed is limited by the employed modulator but could reach 1 GHz for the existing system with >10GHz speed easily achievable (see FIGURE 11). The quality of the single photon source can be further improved by better spectral filtering and by employing a lower QD density sample. In this case the team did not develop an external, bulky, frequency conversion element that couples 1550 nm excitation to a QD at ~900 nm, but instead frequency conversion is done *in situ*, inside the same nanocavity that is used for single photon extraction.

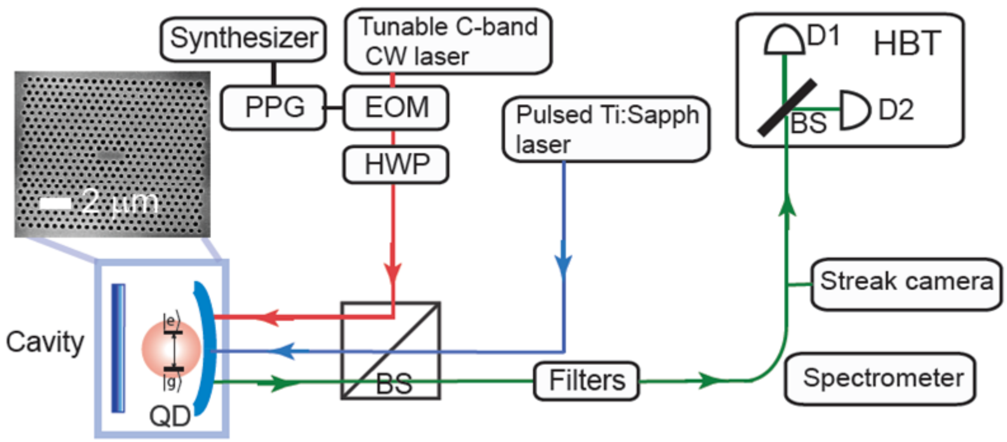

FIGURE 10

Experimental setup for triggered generation of single photons. A tunable C-band laser is modulated by an electro-optic modulator driven by a pulse pattern generator, which receives an external clock signal from a synthesizer. The laser polarization is adjusted to match that of the cavity by a half wave plate (HWP). Pulses incident on the cavity via a non-polarizing beamsplitter (BS) excite quantum dots by above band absorption of laser pulses upconverted by second harmonic generation in the surrounding GaAs matrix. Emission from the dot is spectrally filtered, then analyzed by either a Hanbury Brown and Twiss (HBT) setup for photon correlation measurements or a spectrometer. Inset shows scanning electron microscope image of photonic crystal cavity.

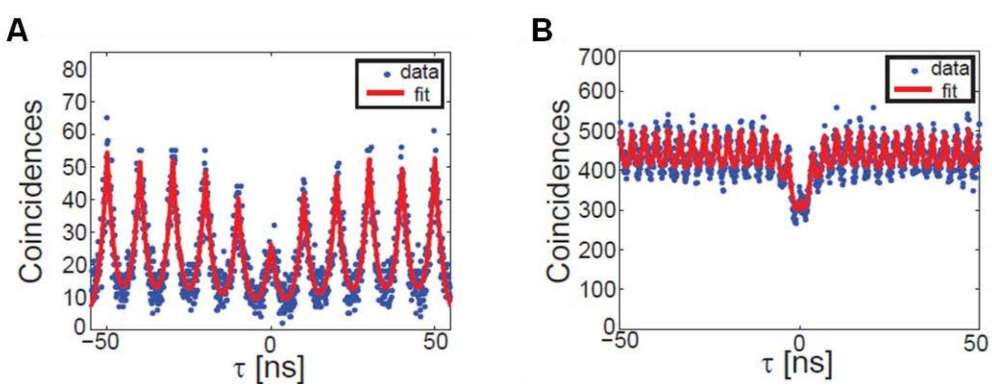

FIGURE 11

Photon correlation measurement of quantum dot emission. The data plots display (A) the photon correlation measurement for 100 MHz repetition rate with 20% duty cycle, and (B) the photon correlation measurement for 300MHz repetition rate with a 50% duty cycle.

H. All-Electrical Control of Single Spins in Semiconducting Nanowire Quantum Dots

Professor Jason Petta, Princeton University, PECASE Award

The goal of this PECASE is to develop an experimental platform that allows "all-electrical" control of spin for quantum information processing. Single-spin control has been achieved using conventional magnetic resonance, but this method has at least two drawbacks: (i) the ac magnetic fields achieved are small, and (ii) the ac magnetic fields are difficult to localize, which limits the ability to address single spins without affecting neighboring spins. In this project, all-electrical control is being achieved using electrically driven spin resonance, where an ac electric field is applied to a depletion gate on an indium arsenide (InAs) nanowire quantum dot. The spin-orbit interaction converts the applied ac electric field into an effective ac magnetic field, resulting in single spin rotations. InAs wires are utilized due to the larger g-factor and shorter spin-orbit length, which will potentially improve speed of operation.

During FY10, InAs nanowires were fabricated with low defect densities and high mobilities. This is a critical step in creating controllable quantum dots in the wires and confining single electrons. InAs and InP nanowires have been synthesized with controllable lengths and diameters. Back-gated field effect transistors have been fabricated and demonstrated nanowire mobilities of 18,000 cm^2/Vs that are among the highest reported in the literature. Top gated and bottom gated nanowire quantum dots have been fabricated and Coulomb blockade has been observed at milli-Kelvin temperatures. The few-electron regime in a single quantum dot has been demonstrated. The g-factor for a single spin has been extracted by measuring the Zeeman splitting as a function of magnetic field. The simplest spin-physics accessible in a single quantum dot is the observation of Zeeman splitting and determination of the electron g factor. This has been demonstrated this in several single InAs nanowire quantum dot samples (see FIGURE 12). Electron g factors have been measured for several different samples and values in the range of 5-10 have been found. These high electron g factors are encouraging for future coherent control of spins.

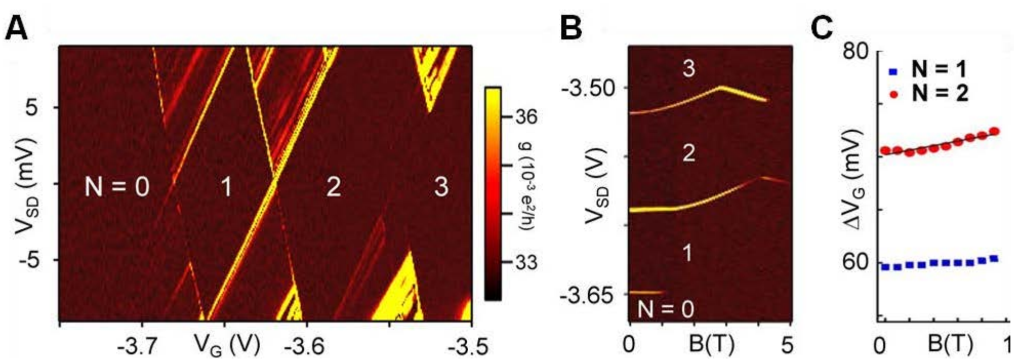

FIGURE 12

Coulomb blockade in InAs quantum dots. (A) The first few Coulomb diamonds for an InAs nanowire single quantum dot are shown, with (B) the zero bias peaks shift with applied magnetic field due to Zeeman splitting. (C) The extraction of the peak positions gives an experimental determination of the electron g factor.

Double quantum dots in InAs nanowires using a "top-gated" approach have also been demonstrated. Device fabrication consists of first defining low resistance ohmic contacts on individual nanowires, then fabricating very fine "finger" gates that rest directly on the nanowire. By eliminating the etch step before depositing the top-gates, the native oxide which forms on the nanowire surface is used as a gate dielectric. The charge stability diagrams of these quantum dots measured at milli-Kelvin temperatures are shown in FIGURE 13. These double quantum dots are an important step towards demonstrating single and two qubit gates with all-electrical control.

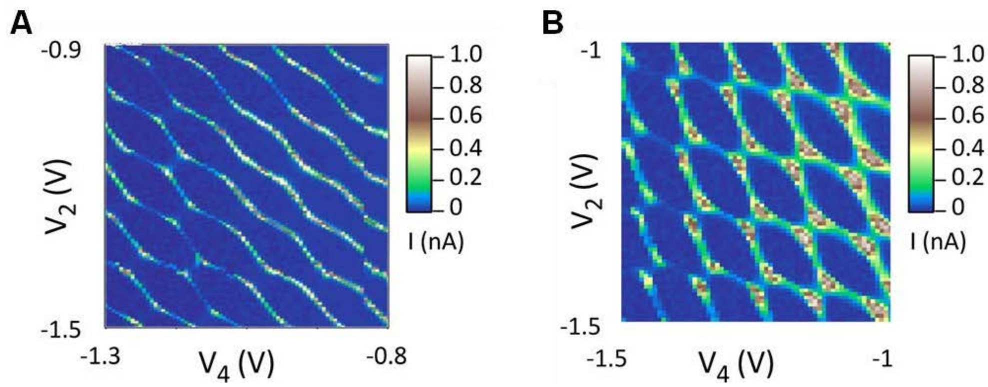

FIGURE 13

Current measured by an InAs nanowire double quantum dot at 30 mK. (A) The gate voltages have been selected to create two strongly coupled quantum dots, while (B) a different selection of gate voltages allows the coupling between the two quantum dots to be lowered.

I. Weak Values and Quantum Amplification Beyond Standard Shot Noise Limit

Professor Andrew Jordan, University of Rochester, Single Investigator Award

The goal of this project is to explore theory and experiments in weak values, quantum amplification, and their relationship to metrology. Professor Andrew Jordan and co-PI Professor John Howell have made significant progress toward this objective in FY10.

First, a method of amplifying small beam deflections using weak values was demonstrated. The amplification is independent of the source of the deflection. In this experiment a small mirror deflection in a Sagnac interferometer provides the beam deflection. Tuning the interferometer and monitoring the resulting small amount of light exiting the interferometer dark port achieved weak value amplification factors of over 100. The weak value experimental setup, in conjunction with a lock-in amplifier, allows the measurement of 560 frad of mirror deflection that is caused by 20 fm of piezo actuator travel.

Second, a detailed analysis was made of the signal-to-noise for the beam deflection measurement. The analysis showed that while this method does not beat the ultimate limit for a beam deflection measurement, it does have a number of improvements over other schemes: (i) the reduction in technical noise, (ii) the ability to use high power lasers with low power detectors while maintaining the optimal signal noise reduction (SNR), and (iii) the ability to obtain the ultimate limit in deflection measurement with a large beam radius. Additionally while weak values can be understood with a classical wave analysis, the SNR in a deflection measurement requires a quantum mechanical understanding of the laser and its fluctuations. It is interesting to note that interferometry and split detection have been competing technologies in measuring a beam deflection. In this study the combination of the two technologies was shown to lead to an improvement that cannot be observed using only one (*e.g.*, measurements of the position of a large radius laser beam with weak value amplification allows for better precision than with a quantum limited system using split detection for the same beam radius). Potential applications that could take advantage of this setup include measuring the surface of an object by replacing the piezo actuator with a stylus such as with atomic force microscopy and measuring frequency changes due to a dispersive material such as in Doppler anemometry.

Third, the measurement of a relative phase shift between two paths in an interferometer was made and amplified using a split-detection method. Furthermore this method is comparable to the sensitivity achievable using balanced homodyne techniques, yet only one output port of the interferometer is measured. These weak value type experiments have the added benefit of reducing technical noise.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned to external organizations and customers.

A. Commercial Off-the-shelf Ultracold Atom Research Device

Investigator: Dana Anderson, University of Colorado, DARPA Award
Recipient: Various DoD Laboratories

As a result of research supported by the DARPA guided Bose-Einstein Condensate Interferometry (gBECi) program, co-managed by the ARO Physics Division, Professor Anderson's start-up company, ColdQuanta, has utilized gBECi advances to develop the first commercial off-the-shelf (COTS) ultracold atom research device. ColdQuanta now provides small kits for generating magneto-optical traps (MOTs) and Bose condensed gases for scientific research. These compact systems are designed for educational institutions and research groups working on cold atoms and provide an alternative to the organizations constructing larger, less-efficient systems (see FIGURE 14).

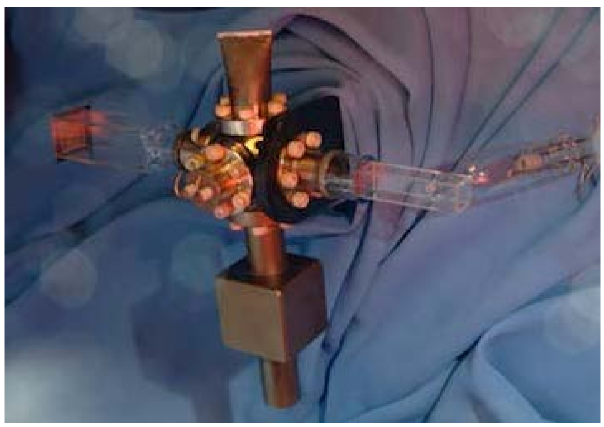

FIGURE 14

Off-the-shelf ultracold atom research device. Available through ColdQuanta, Inc., this device, based on efforts supported through ARO under the DARPA gBECi program, is designed for educational institutions and research groups working on cold atoms. The device eliminates the need for these researchers to invest their manpower in the construction of larger, less-efficient systems.

Several DoD laboratories, including ARL and AFRL, are currently testing and utilizing these devices in a effort to maximize their manpower and they are using them to supplement a myriad of research areas, including atom interferometers for precision navigation. It is believed that these compact sources for coherent atoms, much like their optical counterpart the laser, will reduce much of the effort, time and cost associated with the construction of a compact atom sources.

B. Attosecond Physics

Investigator: Shuting Lei, Kansas State University, MURI Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

Attosecond physics promises to open new doors in optics, from pulse shaping to spectroscopy. Based in part on the research results in attosecond physics achieved through the MURI, Dr. Paul Pellegrino of ARL-SEDD is setting up a femtosecond laser system in his laboratory to carry out ultrashort spectroscopy experiments. Researchers from the MURI team visited Dr. Pellegrino's laboratory and set up a femtosecond laser, which is the first step to achieving and using attosecond pulses for subsequent experiments. The laser system will be used for driving ARL-SEDD research capabilities to the attosecond regime, which will enable sensitivity in spectroscopic detection/classification of substances.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however some ARO-funded research efforts are on the verge of important achievements. This section describes the anticipated FY11 scientific accomplishments for several projects.

A. Ultracold Quantum Chemistry
Professor David Demille, Yale University

Ultracold quantum chemistry is new field of scientific study recently demonstrated in a pivotal 2010 publication[3]. In this remarkable paper, Professor Jun Ye formed quantum molecules at ultracold temperatures and measured the reaction rates. At nano-Kelvin temperatures, chemical reactions are governed by quantum mechanics and the results are radically different than classical chemistry. Models of billiard balls colliding are no longer appropriate and instead, a wavelike picture is required to describe the reactions. Ultracold molecules can react with each though their inter-particle distance is relatively large and there is little movement in the system. Also the reactions are now heavily dependent on spin orientation, interaction strength, and correlations making them a robust testbed for a variety phenomenon.

These two scientific accomplishments in the atomic, molecular, and optical physics community have demonstrated the ability to create ultracold molecules, which are the required ingredient to perform ultracold quantum chemistry. In classical chemistry many of the reactions that occur are governed primarily by the kinetic energy of the samples. However when this kinetic energy is not present (*i.e.*, the samples are ultracold) quantum properties can govern the reactions. In addition these ultracold molecules can have their orientation precisely controlled with external fields allowing novel reactions to occur that are not present at the energies of classical chemistry. It is anticipated that this research will lead to the discovery of the role of quantum effects in chemical reactions.

B. Attosecond Physics
Professor Shuting Lei, Kansas State University

Attosecond pulses are poised to open a new world of physics and applications in chemistry, biology, and materials science (refer to Section II-C.4). Molecular orbitals, due to the way they distort the wave function of the electron that was removed and returned from a molecule, can be "seen" and orbitals have already been mapped for simple molecules. A new level of spectroscopy is also expected to result from the attosecond pulses, as well as improved techniques in beam shaping. In quantum control, the precise profile of a laser beam is established, sometimes by adaptive algorithms, to enable it to spectroscopically interrogate an unknown substance, possibly from a distance. With the exquisite control afforded by as timing, it may be possible to detect explosive or other residue from significant standoff distances. Research at Kansas State University has already resulted in confirmation of the generating attosecond pulses down to 120 attoseconds (refer to Section III-F). It is anticipated that the research team will confirm a pulse of 65 attoseconds in duration. It is also anticipated that the team will develop a new kind of streak camera that can measure pulses as short as 25 attoseconds. If succesfful, their results may mark the beginning of a new field that may be called atto-optics.

C. Charged Quantum Dots Strongly Coupled to a Photonic Crystal Cavity
Professor Jelena Vuckovic, Stanford University

Several accomplishments in photonic systems are anticipated based on ongoing research in quantum information science. It is anticipated that this research will lead to the optically-initialized spin of a charged quantum dot inside a photonic crystal cavity. If successful this would be the first demonstration of a stationary qubit

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[3] S. Ospelkaus, K.-K. Ni, D. Wang, M.H.G. de Miranda, *et al*. (2010). Quantum-state controlled chemical reactions of ultracold potassium-rubidium molecules. Science 327, 853-857.

(memory) node coupled to a photon (flying qubit) via an optical interface. Experiments are planned to demonstrate selective quantum dot charging, high-Q doubly degenerate cavities and mapping of the photon state to the quantum dot state. Previous accomplishments have shown coupling of a 1.5 µm photon to a 900 nm quantum dot. This success sets the framework to demonstrate the reciprocal approach, where 900 nm emission from a quantum dot is converted to a 1550 nm photon using a process such as difference frequency generation. A key advantage of this approach is the elimination of an external, bulky, frequency conversion element, with frequency conversion done *in situ* (*i.e.*, inside the same nanocavity that is used for cavity quantum electrodynamics (QED).

D. All-electrical Control of Electron Spin in Nanowire Quantum Dots
Professor Jason Petta, Princeton University

In the area of nanowire research as a platform for qubits, key demonstrations of all-electrical control of electron spin are anticipated. Synthesis of single composition nanowires is now well developed (*e.g.*, InAs and InP). The next step is to understand the role the surface has in determining sample quality. For example the high mobilities obtained in GaAs two-dimensional electron gases are made possible by burying the electrically active layer more than 100 nm below the surface of the wafer and by using remote doping. It is anticipated that the use of core-shell wires to obtain quantum dots will be achieved in FY11 where the active core is protected from the surface by the shell. Previous accomplishments have shown that the top-gated approach suffers from hysteresis. Hysteresis problems have been largely absent in bottom-gated nanowire samples.

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